Valley caloritronics in a photodriven hetero-junction of Dirac materials

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We consider a lateral hetero-junction where the left and right leads are made of monolayer graphene and the middle region is made of a gapped tilted Dirac material (borophene or quinoid graphene) illuminated with circularly polarized radiation. The tilt parameter makes the band gap indirect and smaller in magnitude as compared to Dirac materials without tilt. The radiation makes the band gaps valley-dependent which show their signatures as valley polarized transport. In a systematic framework, we compute the valley polarized electrical conductance, thermal conductance, thermopower and the figure of merit of this junction device and study the interplay among the valley index $\zeta$, a gap parameter $\eta$ and the tilt parameter $v_t$, and finally compare the results with the corresponding charge properties in details. For non-zero $\eta$, the valley polarized electrical conductance attains a peak and then asymptotically vanishes with increase in chemical potential. The gap parameter enhances all the valley polarized properties, the charge thermopower and charge figure of merit, but reduces the charge conductances (electrical and thermal). Furthermore, the tilt parameter reduces the effective transmission of carriers through the junction, thereby diminishing all the charge and valley polarized quantities. As the gaps in the dispersion can be adjusted by experimental setup, a tunability of this junction with regard to its thermoelectric properties may be experimentally achieved.

I. INTRODUCTION

Thermoelectric materials have attracted immense interest in energy efficient device applications [113]. High thermopower, high electrical conductivity and low thermal conductivity are desirable properties of a highly efficient thermoelectric device. The efficiency of power generation in such devices depends on the interplay between their electronic and thermal performances and it is characterized by a dimensionless quantity called figure of merit, $ZT = S^2\sigma T/\kappa$, where $\sigma$, $\kappa$ and $S$ denote electrical conductivity, thermal conductivity and Seebeck coefficient (thermopower), respectively, with $T$ being the absolute temperature. In bulk materials, the factors in the expression of $ZT$ are mutually coupled in such a way that it is difficult to control them independently, and hence improve $ZT$. The techniques used to improve the figure of merit rely on enhancing the power factor ($\sigma S^2$) and lowering the thermal conductivity. One of the important proposals is nanostructuring of materials which enhances thermoelectric efficiency due to the sharply peaked density of states (DOS) of the carriers in low-dimensional materials [114]. Another useful method is the engineering band structure [15, 16] in conjunction with nanostructuring to lower the thermal conductivity. Further, the use of semi-metals with large electron-hole asymmetry can enhance the thermoelectric coefficients [17].

Advancements in fabrication technologies have opened up new ways of exploring two-dimensional materials for thermoelectric applications [7, 11]. Since the realization of graphene [18, 19] there have been numerous experimental and theoretical studies of quasi-2D materials supporting Dirac cones such as silicene [20], germanene [21], and MoS$_2$ [22]. Recently, there has been immense interest in synthesis of 2D crystalline boron structures, generally known as borophene [23–25]. It is a zero gap semiconductor with tilted anisotropic Dirac cones [26, 27], which can be thought of as topologically equivalent to the quinoid graphene [28, 29]. Optical [30], magneto-transport [31], collective modes [32], Floquet states [33] and thermoelectric properties [34] of bulk borophene have been studied extensively. Besides, a very recent success of integrating dissimilar two-dimensional (2D) materials [34] which is essential for nano-electronic applications, has opened a new direction for studying the thermoelectric in junction devices of different materials. In Ref. [35], the authors have reported the covalent lateral stitching of borophene-graphene, resulting in rare realization of 2D lateral hetero-structure where the lateral interfaces are atomically sharp despite imperfect crystallographic lattice and symmetry matching.

The concept of valleytronics, similar to spintronics [36–38], is becoming popular in recent past [39, 42]. In valleytronic devices, the information is carried by the valley degree of freedom of the charge carriers. The generation of valley polarization and optically excited valley-polarized current in various materials have been studied theoretically as well as experimentally [43–46]. The harnessing of internal degrees of freedom like spin/valley of the charge carriers by applying thermal gradient and the associated phenomena are called spin/valley caloritronics.

Motivated by the above discussion, we study the thermoelectric effects of a nano-junction system where the left and right electrodes are made of graphene and the middle region is made of 2D Dirac material having tilted anisotropic Dirac cones, such as borophene or quinoid graphene. The middle region has different onsite energies on the two sublattices and is subjected to circularly...
polarized electromagnetic radiation. It results in valley dependent bands at the two Dirac points and hence a valley dependent transmission probability. Thus, in analogy with the spin-caloritronic studies, thermally activated quantum transport of valley degree of freedom of the charge carriers can be achieved. One of our goals is to study thermally driven valley polarized properties, known as valley caloritronics and compare them with that of the charge caloritronics in detail.

This paper is organized as follows. In Sec. (II), we present basic information of the lateral junction along with the calculation of the transmission probability through the junction. In Subsec. (II B), we present the theory of thermoelectricity. All the numerical results and their corresponding discussions are presented in Sec. (III). Finally, we conclude and summarize our main results in Sec. (IV).

II. MODEL AND THEORETICAL METHODS

Here, we first present the essential information of the junction characterized by the quasi-ballistic transport, along with the calculation of the transmission probability as a function of incident energy and incident angle. Later we present general description of thermoelectric coefficient (Seebeck coefficient), electrical conductance, thermal conductance and figure of merit for any junction device. The discussions in Sec. (II B) are applicable to any junction characterized by the quasi-ballistic transport.

A. Basic information of the junction

We consider a two-dimensional junction system placed on the xy plane at room temperature as shown in Fig. 1. The left (x < 0) and right (x > L) leads are made of graphene sheets, while the middle region (0 < x < L) is made of a 2D material hosting tilted anisotropic Dirac dispersion (can be considered as borophene or quinoid graphene) with a mass gap at low energy. Further, it is assumed that the middle region is subjected to a circularly polarized electromagnetic radiation where the photon energy satisfies the off-resonant condition, i.e., the photon energy is much higher than the band width of the undriven lattice in the middle region of the system. The off-resonant circularly polarized light induces a gap in the energy dispersion.

The Hamiltonian for the charge carriers in graphene sheet in the vicinity of the Dirac points is given by

\[ H_G = \zeta \hbar v_F (\sigma_x k_x + \zeta \sigma_y k_y), \]  

where \( \zeta = \pm \) denotes two independent Dirac points, \( v_F = 10^6 \text{ m/s} \) is the Fermi velocity, \( \sigma_x, \sigma_y \) are the Pauli matrices denoting the sublattice degrees of freedom. The corresponding energy dispersion of the Hamiltonian in Eq. (1) is given by \( E_{\lambda}(k) = \lambda \hbar v_F k \), independent of the valley pseudo-spin \( \zeta \), where \( \lambda = \pm \) denotes the conduction and valance bands, respectively. The corresponding eigenfunctions are given by \( \Psi^\lambda_\zeta (r) = e^{i \phi} (1, \zeta \lambda e^{i \delta} \sigma^T) \), where \( \phi = \tan^{-1} k_y / k_x \) and \( T \) denotes the transpose operation.

The effective Floquet Hamiltonian, describing the charge carriers of the middle region subjected to circularly polarized electromagnetic radiation, in the vicinity of the two independent Dirac points can be written as (see Appendix),

\[ H_B = \zeta \hbar [v_x \sigma_x \sigma_x + \zeta v_y q_y \sigma_y + v_t \sigma_0] + \Delta \zeta \sigma_z. \]  

Here, \( \sigma_0 \) is the 2 \times 2 identity matrix and \( \Delta \zeta = M + \zeta \Delta \) is the net valley-dependent mass resulting from the valley-dependent photoinduced mass \( \Delta \) and onsite energies on the two sublattices \( \pm M \). We define a dimensionless parameter \( \eta = M / \Delta \) such that \( \Delta \zeta = \Delta (\eta + \zeta) \). It is worth noting that the photoinduced mass \( \Delta = (e A_0)^2 v_x v_y / (\hbar \omega) \) can be tuned experimentally. Here, \( (v_x, v_y, v_t) \) are the direction dependent velocities where \( v_t \) (tilt parameter) is responsible for the tilt in energy dispersion. The values of these velocities for borophene are \( v_x = 0.86 v_F, v_y = 0.69 v_F \) and \( v_t = 0.32 v_F \). The energy dispersion and the corresponding wave functions associated with the Hamiltonian in Eq. (2) are given by

\[ E_{\lambda,\zeta}(q) = \zeta \hbar v_t \sin \theta + \lambda \sqrt{\Delta_\zeta^2 + [\hbar \Lambda(\theta) \sigma^T]^2}, \]  

and

\[ \Psi^\lambda_\zeta (r) = \frac{1}{\sqrt{2}} \left( \frac{\zeta \hbar \Lambda(\theta) \sigma^T}{\Delta_\zeta + \lambda \sqrt{\Delta_\zeta^2 + [\hbar \Lambda(\theta) \sigma^T]^2}} \right). \]
where \( \delta = \tan^{-1}(v_yq_y/v_xq_x) = \tan^{-1}(\delta_0 \tan \theta) \) with \( \delta_0 = v_y/v_x, \theta = \tan^{-1}(q_y/q_x) \) and \( \Lambda(\theta) = \sqrt{v_y^2 \cos^2 \theta + v_x^2 \sin^2 \theta} \) having dimension of velocity.

The band structure of borophene in the two valleys with valley-dependent masses is shown in Fig. (2) for \( \eta = 0.5 \). The system is an insulator with valley-dependent indirect band gaps \( \gamma_\zeta \). The shift \( \chi_\zeta \) between maxima of valence band and minima of conduction band in both the valleys is along the \( q_y \) axis. The magnitude of the indirect gaps and the shifts are given as

\[
\gamma_\zeta = 2\Delta_\zeta \sqrt{1 - \frac{v_y^2}{v_y^2}}, \quad \chi_\zeta = \frac{2v_1\Delta_\zeta}{h\nu_y\sqrt{v_y^2 - v_t^2}}.
\]

Equation (5) reveals that the band gaps reduce due to tilt and decrease monotonically with \( v_t \) for \( v_t < v_y \) while the shifts corresponding to the gaps increase. For \( \eta > 0 \), the band gap at \( K' \) valley is smaller than at \( K \) valley. So, the effective band gap of the system is \( \gamma_\zeta \). The direct gaps at the original Dirac points are equal to \( 2\Delta_\zeta \).

The middle region can be reduced to a gapped graphene by setting \( v_t = 0 \) and \( v_x = v_y = v_F \), so that the junction becomes a graphene/gapped-graphene/graphene junction. If the Fermi energy lies in the gap, the middle region behaves like a topological insulator when \( M < \Delta \), otherwise it is a trivial insulator.

In the topological insulating state, the edge states contribute to the transport quantities. Since our system is kept at room temperature, the contribution from the bulk states would dominate over the edge states contribution.

Suppose an electron from the left lead is injected with an energy \( \epsilon \) and incident angle \( \phi \). The different processes that take place at the interfaces are depicted in Fig. (1). The wave functions in the three different regions, \( \Psi_1(x,y), \Psi_2(x,y) \) and \( \Psi_3(x,y) \) will have the same \( y \)-dependence: \( \Psi_i(x,y) = \Psi_i(x)e^{iq_yy} \) with \( i = 1, 2, 3 \). The wave functions, \( \Psi_1(x), \Psi_2(x) \) and \( \Psi_3(x) \) for the three different regions for \( A \) and \( B \) sublattices can be written in the following forms: for \( x < 0 \),

\[
\Psi_1^x(x) = \left( \begin{array}{c} e^{i\kappa_1 x} \\ \zeta e^{i\kappa_1 x+i\zeta \phi} \end{array} \right) + r_\zeta \left( \begin{array}{c} e^{-i\kappa_1 x} \\ -\zeta e^{-i\kappa_1 x-i\zeta \phi} \end{array} \right),
\]

for \( 0 < x < L \)

\[
\Psi_2^x(x) = a_\zeta \left( \begin{array}{c} e^{i\kappa_2 x} \\ \zeta e^{i\kappa_2 x+i\zeta \phi} \end{array} \right) + b_\zeta \left( \begin{array}{c} e^{-i\kappa_2 x} \\ -\zeta e^{-i\kappa_2 x-i\zeta \phi} \end{array} \right)
\]

and for \( x > L \)

\[
\Psi_3^x(x) = t_\zeta \left( \begin{array}{c} e^{i\kappa_3 x} \\ \zeta e^{i\kappa_3 x+i\zeta \phi} \end{array} \right).
\]

Here the expression for \( p_\zeta \) is given by

\[
p_\zeta = \frac{h\nu \Lambda(\theta)}{\Delta_\zeta + \sqrt{\Delta_\zeta^2 + [h\nu \Lambda(\theta)]^2}}.
\]

The valley dependent reflection amplitude \( r_\zeta \) and the transmission amplitude \( t_\zeta \) are obtained by matching the wave functions at the interfaces \( x = 0 \) and \( x = L \):

\[
\Psi_1^x(x = 0) = \Psi_2^x(x = 0); \Psi_2^x(x = L) = \Psi_3^x(x = L).
\]

From the above conditions, the valley-dependent transmission probability \( T_\zeta(\epsilon, \phi) = |t_\zeta(\epsilon, \phi)|^2 \) is obtained as

\[
T_\zeta(\epsilon, \phi) = \frac{4p_\zeta^2 \cos^2 \phi (1 + \cos 2\delta)}{(2\sqrt{2}p_\zeta \cos \phi \cos \delta)^2 + [1 + p_\zeta^2 - 2p_\zeta \cos(\phi - \delta)][1 + p_\zeta^2 + 2p_\zeta \cos(\phi + \delta)][1 - \cos(2qL \cos \theta)]}.
\]

Here, it should be noted that there is no mechanism present in the junction that mixes states of opposite valleys. The system can be reduced to a gapless single graphene sheet by setting \( \Delta_\zeta = 0 \), \( v_t = 0 \) and \( v_x = v_y = v_F \). In this limiting case, it can be easily checked that \( T_\zeta(\epsilon, \phi) = 1 \). To understand the behavior of the transmission probability \( T_\zeta(\epsilon, \phi) \) for different condi-
FIG. 3. Transmission probability $T_{\zeta}(\epsilon, \phi)$ as a function of incident angle $\phi$ for (a) $\eta = 0.5$, (b) $\eta = 2$ when $v_t = 0, v_x \neq v_y$.

FIG. 4. Transmission probability $T_{\zeta}(\epsilon, \phi)$ as a function of incident angle $\phi$ for (a) $\eta = 0.5$, (b) $\eta = 2$ when $v_t = 0, v_x = v_y = v_F$.

FIG. 5. Transmission probability $T_{\zeta}(\epsilon, \phi)$ as a function of incident angle $\phi$ for (a) $\eta = 0.5$, (b) $\eta = 2$ when $v_t \neq 0, v_x \neq v_y$.

FIG. 6. $T_{\zeta}(\epsilon)$ vs $\epsilon$ for (a) $\eta = 0.5$, (b) $\eta = 2$ when $v_t \neq 0, v_x = v_y = v_F$.

FIG. 7. $T_{\zeta}(\epsilon)$ vs $\epsilon$ for (a) $\eta = 0.5$, (b) $\eta = 2$ when $v_t \neq 0, v_x = v_y = v_F$.

figures, plots for $T_{\zeta}(\epsilon, \phi)$ as a function of the incident angle $\phi$ for a fixed energy $\epsilon = 0.5$ eV and $L = 50$ nm are shown in Figs. (3), (4) and (5).

Figures (3) and (4) show plots of $T_{\zeta}(\epsilon, \phi)$ as a function of $\phi$ for (i) $v_t = 0, v_x \neq v_y$ and (ii) $v_t = 0, v_x = v_y = v_F$ for two values of $\eta$ with $\Delta$ fixed at 0.05 eV. On the other hand, Fig. (5) shows plot of $T_{\zeta}(\epsilon, \phi)$ as a function of $\phi$ for $v_t \neq 0, v_x \neq v_y$. All the figures show that the transmission probability is close to unity around the normal incidence ($\phi \to 0$) for both the valleys. This is manifestation of perfect tunneling when incident wave vector is normal to the interface. Figure (3) shows that the transmission is allowed over the full range of incident angle ($-\pi/2 \leq \phi \leq \pi/2$), whereas for Fig. (4), the transmission is restricted below the lower critical angle and above the upper critical angle. Further, in Fig. (5), the transmission probability for $\zeta = +/-$ ceases to zero above/below some critical incident angles. This is because of $\sin \theta > 1$, as shown in the inset of the Fig. (5), for which above or below the critical angles the wave vector in the middle region becomes complex which leads to evanescent wave. Figures (4) and (5) reveal that the allowed range of incident angle for $\zeta = -1$ is bigger than that of the $\zeta = 1$, as for the latter one, the band gap is wider. It is clear that the value of critical angles depend on all the three velocities $v_x, v_y$ and $v_t$. Similar critical angles exist in other semiconductor junction devices [48, 49].

We define the effective transmission coefficient for current along $x$ direction at a given energy $\epsilon$ as $T_{\zeta}(\epsilon) = \int_{-\pi/2}^{\pi/2} T_{\zeta}(\epsilon, \phi) \cos \phi d\phi$. In Figs. (6), (7), $T_{\zeta}(\epsilon)$ vs $\epsilon$ is
The charge current is given by the formalism in quasi-ballistic regime, the valley-dependent distribution function $f_{\ell}$, where $\phi$ is a function of $\epsilon$. In case of $v_\ell = v_y = v_F$, and $E \gg \Delta_\ell$, the values of the $\phi$ and $\delta$ become equal and $\mu_\ell$ becomes $\sim 1$, which eventually yields the coefficient of $(1 - \cos(2qL \cos \theta))$ to be $\sim 0$ and thus $T_\ell(\epsilon, \phi)$ becomes $\sim 1$ (see Eq. 11) and $T_\ell(\epsilon) \sim 2$. As a result no such noticeable oscillations are obtained (see red curves of Figs. 6 and 7). The physics behind this can be explained using the concept of electron wave interference – when $v_\ell = 0$, $v_x = v_y = v_F$ and $E \gg \Delta_\ell$, the system can be viewed as a single graphene sheet without any barrier. Thus, almost all the incoming electron waves from the left lead get transmitted to the right lead, leaving almost no reflected wave and thereby causing no interference. If the band gap is further increased, the probability of the reflection of electron waves from the interface increases; so the reflected and the transmitted electron waves begin to interfere. This results in oscillations in the transmission probability for $v_\ell = 0$, $v_x = v_y = v_F$ case as well (see blue curves in Figs. 6 and 7). Furthermore, the $K'$ valley has smaller $T_\ell(\epsilon)$ as compared to $K'$ valley. It can be understood using the analogy of transmission through a rectangular potential barrier. If the middle region is considered as a potential barrier with a barrier height $\Delta_\ell$, the transmission probability is smaller for a larger barrier height for the considered range of incident energies above the barrier. Since $\Delta_\ell > \Delta_\ell$, $K$ valley allows lesser transmission than $K'$. The tilted velocity term diminishes $T_\ell(\epsilon)$, as for $v_\ell \neq 0$ the transmission probability as a function of incident angle shows more deviation from 1 compared to $v_\ell = 0$ case (see Figs. 3, 4 and 5). Moreover, the $T_\ell(\epsilon)$ is almost electron-hole symmetric (see Figs. 6, 7) although $v_\ell$ breaks the electron hole symmetry in band structure (see Fig. 2).

Assuming that the graphene leads are independent electron reservoirs, the chemical potential and the temperature of the left/right graphene leads are $\mu_L/R$ and $T_{L/R}$, respectively. The population of electrons at the left/right leads is described by the Fermi-Dirac formalism in quasi-ballistic regime, the valley-dependent charge current is given by

$$I_\ell = \frac{2e}{h} \int_{-\pi/2}^{\pi/2} d\phi \cos \phi \int_{-\infty}^{\infty} N(\epsilon) T_\ell(\epsilon, \phi)(f_L - f_R) d\epsilon, \quad (13)$$

where $N(\epsilon) = W |\epsilon|/(\pi \hbar v_F)$ is the energy dependent number of transverse modes in the graphene sheet of width $W$. The net current is defined as $I_+ = I_+ + I_-$ and the valley polarized current is defined as $I_\ell = |I_+ - I_-|$. Here it has been used that $T_{L/R}(\epsilon, \phi) = T_{R/L}(\epsilon, \phi)$ with $T_{L/R}(\epsilon, \phi)$ the transmission probability of an electron with energy $\epsilon$ and incidence angle $\phi$ from left (right) graphene leads.

The flow of electrons can also transport thermal energy through the junction, which is responsible for the thermal current. The electron’s thermal current is the energy current carried by electrons traveling between leads driven by $dT = T_R - T_L$ and $dV = (\mu_R - \mu_L)/e$. Analogous to the charge current, the electron’s valley resolved thermal current can be written as

$$J_\ell^T = \frac{2}{h} \int_{-\pi/2}^{\pi/2} d\phi \cos \phi \int_{-\infty}^{\infty} N(\epsilon) T_\ell(\epsilon, \phi)(\epsilon - \mu)(f_L - f_R) d\epsilon. \quad (14)$$

Equations (13) and (14) are essential for deriving the different thermoelectric properties in a junction system which are elaborately discussed in the next subsection.

### B. Theory of Thermoelectricity

In this subsection, we present a general formalism of zero-bias electric conductance, thermopower and electron’s thermal conductance in terms of the transmission probability for a lateral junction. Later, we briefly mention about the general expression for thermoelectric figure of merit.

The left and right leads act as independent temperature reservoirs. In absence of any external bias voltage ($V_B$), the chemical potentials of the two leads are taken to be the same as $\mu_L = \mu_R = \mu$. Due to the applied temperature difference ($dT$) between the two leads, there will be a small voltage difference ($dV$) between the leads. The currents induced by $dT$ and $dV$ are given by $(dI_\ell)_T = I_\ell(\mu, T; \mu, T + dT)$ and $(dI_\ell)_V = I_\ell(\mu, T; \mu + e dV, T)$, the currents $I_\ell(\mu, T; \mu, T + dT)$ and $I_\ell(\mu, T; \mu + e dV, T)$ can be calculated from Eq. 13.

Since in an open circuit situation, the current cannot flow, one can write

$$dI_\ell = (dI_\ell)_T + (dI_\ell)_V = 0. \quad (15)$$

Expanding the Fermi-Dirac distribution functions in Eq. 13 and Eq. 15 in the linear response regime, i.e., up to the first order terms in $dV$ and $dT$, one can get the valley resolved Seebeck coefficient $S_\ell$ as

$$S_\ell = \frac{dV}{dT} \bigg|_{dI_\ell=0} = -\frac{L_\ell^{(0)}}{e TL_\ell^{(0)}}, \quad (16)$$

where the kinetic coefficients $L_\ell^{(0)}$ for the quasi-ballistic transport regime are given by

$$L_\ell^{(0)} = \int_{-\pi/2}^{\pi/2} d\phi \cos \phi \int_{-\infty}^{\infty} T_\ell(\epsilon, \phi) N(\epsilon) (\epsilon - \mu)^\alpha (-\partial f/\partial \epsilon) d\epsilon$$

with $\alpha = 0, 1, 2$.

Similar to Ref. 51, we have defined the charge Seebeck coefficient as $S_\ell = (S_+ + S_-)/2$ and using the same
analogy for the spin current, the valley polarized Seebeck coefficient is defined as \( S_{\pm} = |S_{\uparrow} - S_{\downarrow}|/2 \).

As mentioned earlier, the flow of electrons can also transports thermal energy through the junction which is responsible for the thermal current. Analogous to the charge current driven by \( dT \) and \( dV \), the electron’s valley resolved thermal current can be written as

\[
dJ^{el}_{\zeta} = (dJ^{el}_{\zeta})_T + (dJ^{el}_{\zeta})_V,
\]

where \((dJ^{el}_{\zeta})_T = J^{el}_{\zeta}(\mu, T; \mu, T + dT)\) and \((dJ^{el}_{\zeta})_V = J^{el}_{\zeta}(\mu, T; \mu + e dV, T)\). Note that \( dV \) is generated by the Seebeck effect due to the temperature difference \( dT \). Both \( J^{el}_{\zeta}(\mu, T; \mu, T + dT) \) and \( J^{el}_{\zeta}(\mu, T; \mu + e dV, T) \) can be calculated using Eq. (14). Similarly, the electron’s thermal conductance, \( k^{el}_{\zeta} = dJ^{el}_{\zeta}/dT \) has two components:

\[
k^{el}_{\zeta} = (k^{el}_{\zeta})_T + (k^{el}_{\zeta})_V,
\]

where \((k^{el}_{\zeta})_T = (dJ^{el}_{\zeta})_T/dT\) and \((k^{el}_{\zeta})_V = (dJ^{el}_{\zeta})_V/dT\) are the portions of the electron’s thermal conductance driven by \( dT \) and \( dV \) respectively. The electron’s valley resolved thermal conductance can be expressed in terms of the kinetic coefficients \( L^{(\alpha)}_{\zeta} \) as [52][53]

\[
k^{el}_{\zeta} = \frac{2}{\hbar} L^{(2)}_{\zeta} + \frac{2e}{\hbar} L^{(1)}_{\zeta} S^{el}_{\zeta}.
\]

At zero external bias voltage, the valley resolved electrical conductance (charge conductance) \( G_{\zeta} \) arising solely due to \( dT \) can be expressed as

\[
G_{\zeta} = \left. \frac{dJ_{\zeta}}{dV} \right|_{V_B=0} = \frac{2e^2}{\hbar} L^{(0)}_{\zeta}.
\]

The total charge and thermal conductance are defined as \( G_c = G_+ + G_- \) and \( k^{el}_{\zeta} = k^{el}_{\uparrow} + k^{el}_{\downarrow} \). Similar to the valley current, the valley polarized charge conductance and the valley polarized thermal conductance can be defined as \( G_v = |G_+ - G_-| \) and \( k^{el}_{\zeta} = |k^{el}_{\uparrow} - k^{el}_{\downarrow}| \) respectively, where \( G_{\pm} \) and \( k^{el}_{\pm} \) are the valley resolved charge conductance and valley resolved electrical thermal conductance.

One of the challenges in fabricating thermoelectric devices is to obtain optimal conditions which ensure the operation of the device with maximum power at the best possible efficiency. The efficiency of the system depends upon a quantity called as figure of merit \( ZT_e \) which is defined by

\[
ZT_e = \frac{S^2_e G_e}{k^{el}_{\zeta} + k^{ph}_{\zeta} T},
\]

where \( S_e \) is charge Seebeck coefficient, \( G_e \) is the charge conductance, \( k^{el}_{\zeta} \) is the thermal conductance of the carriers, \( k^{ph}_{\zeta} \) is phonon’s thermal conductance owing to the involvement of lattice structure and \( T \) is the absolute temperature. In this context we would like to mention that the Debye temperature in borophene has a high value about 2000 K [54][55] due to the strong bonding. Further, graphene has also a higher Debye temperature \( \theta_D = 2300 \) K, approximately an order of magnitude higher than for typical metals. Thus, the room temperature (300 K) is safely assumed to be low with respect to high Debye temperatures of borophene and graphene. Due to this reason, the phonon population is expected to be low at room temperature, which diminishes the possibility of phonon-phonon inelastic scattering events. Henceforth we neglect the phonon’s contribution in thermal conductance. Here also, we define a quantity named valley polarized figure of merit, \( ZT_v = \frac{S^2_G}{k^{el}_{\zeta}} T \) using the concept of spin polarized figure of merit in Ref. [51].

### III. RESULTS AND DISCUSSION

Here we present numerical results of different thermoelectric properties of the junction subjected to the Floquet radiation. For our numerical analysis, we choose the parameters \( v_s = v_x = v_F, v_t = 0.32 v_F \) and \( \Delta = 0.05 \) eV. The dimensionless parameter, \( \eta = M/\Delta \) is varied in the range \( [0 : 1.5] \). Temperature of the junction is maintained at \( T = 300 \) K. The dimension of system is taken as \( (L, W) = (50, 30) \) nm.

#### A. ELECTRICAL CONDUCTANCE

(a) Dependence on chemical potential: We start by analyzing the behavior of the electrical conductance as a function of the chemical potential \( \mu \) for different values of \( \eta \) as shown in Fig. (8). The charge conductance increases monotonically with increase in \( |\mu| \). This is primarily due to the increase in the number of available conducting channels \( N(\epsilon) \) in the leads with increase in \( |\epsilon| \). On the other hand, the valley polarized conductance has peaks at \( \pm \mu_p(\eta) \). This feature is also present when the middle region is gapped graphene with unequal masses \( \Delta \zeta \) in the two valleys, indicating that tilt
in dispersion is not responsible for the peaks. The appearance of peaks can be explained using an analogy with transmission through a rectangular barrier. For gapped graphene, the dispersion can be approximated as \( E_\zeta \approx \Delta_\zeta + \frac{k^2 q^2}{2\Delta_\zeta/v_F^2} \) near the band minima/maxima. So, the middle region can be viewed as a potential barrier with valley-dependent barrier heights \( (V_\zeta = \Delta_\zeta) \) and effective masses \( (m_\zeta = \Delta_\zeta/v_F^2) \). The rate of increase of transmission \( T(\epsilon) \) with \( \epsilon \) for smaller mass \( (\Delta_-) \) is higher than that with larger mass \( (\Delta_+) \) for energies just above the barrier (see Figs. (6) and (7)). Since \( G_\zeta(\epsilon) \) is proportional to \( T_\zeta(\epsilon) \), \( G_+ \) increases slowly with \( \mu \) resembling a quadratic growth, while \( G_- \) rises sharply resembling almost a linear growth due to smaller mass. For higher value of \( |\mu| \), the effect of mass in the dispersion becomes negligible in both the valleys which results in almost similar variation of their conductances with \( |\mu| \). Due to this nature, the valley polarized conductance \( (|G_+ - G_-|) \) increases with \( |\mu| \) initially, attains a maximum (peak) and then decreases asymptotically to zero at higher \( |\mu| \). As expected, the charge conductance is always greater than the valley conductance for a given \( \eta \).

(b) Dependence on gap parameter: In \( K \) valley \( (\zeta = 1) \), \( \Delta_+ \) monotonically increases with \( \eta \), thereby reducing critical angles and hence the number of conducting channels and \( T_\zeta(\epsilon) \) (see Figs. (6) and (7)). It results in lowering of the charge conductance \( G_+ \). However, the gap varies non-monotonically with \( \eta \) in \( K' \) valley \( (\zeta = -1) \). In this valley, \( |\Delta_-| \) starts decreasing with increase in \( \eta \) (for \( \eta < 1 \), vanishes at \( \eta = 1 \) and starts to increase again with \( \eta \) for \( \eta > 1 \). Thus, depending on the strength of \( \Delta_- \), \( G_- \) initially increases with \( \eta \) for \( \eta < 1 \), attains maximum value at \( \eta = 1 \) and then starts to decrease with increasing \( \eta \). Depending on \( G_\zeta \)'s behavior as a function of \( \eta \), the total conductance \( G_\zeta \) shows it nature (Fig. (8a)). The figure reveals that \( G_\zeta \) gets diminished (though the change is small, but noticeable) with increasing \( \eta \), away from the low chemical potential regime. Near the low chemical potential region, there are crossovers in the conductance plot. The valley resolved properties arise due to the term \( \Delta_\zeta = M + \Delta \). For \( \eta \to 0, \Delta_\zeta \to \zeta \Delta \) does not yield any valley resolved properties, since in Eq. (9), \( p_\pm \) becomes \( 1/p_- \) which eventually yields \( T_\zeta(\epsilon, \phi) = T_\zeta(\epsilon, -\phi) \) (see Eq. (11)). On integration over the full range of incident angle, both the valleys gain the same value of transmission at a given energy. Thus, \( \eta \) can be seen as a measure of mismatch between the two valleys. It implies that with increasing value of \( \eta \), the valley conductance should increase which is reflected on Fig. (8b), though there is a crossover between the curves for \( \eta = 0.8 \) and \( \eta = 2 \) near the chemical potential to be zero.

(c) Dependence on tilt parameter: The tilted term diminishes the charge conductance, as \( v_t \) diminishes \( T_\zeta(\epsilon) \). Further, the valley polarized conductance also decreases with \( v_t \), since \( v_t \) diminishes the \( (T_-(\epsilon) - T_+(\epsilon)) \) as well (see Figs. (6) and (7)). It is interesting to note that charge and valley conductances show high degree of electron-hole symmetry despite the fact that the spectrum in the middle region is electron-hole asymmetric due to non-zero \( v_t \). Similar behaviour is shown in bulk borophene [44].

B. SEEBOECK COEFFICIENT

(a) Dependence on chemical potential: The charge and valley Seebeck coefficients \( S_\zeta \) and \( S_\zeta' \) (in units of \( k_B/e \)) as a function of the chemical potential \( \mu \) for various values of \( \eta \) are shown in Fig. (9). The maximum (absolute) thermopower appears at a value of \( \mu \sim \pm 0.04 \) eV, which is roughly independent of \( \eta \). The peak in the thermopower arises due to \( (\epsilon - \mu)(-\frac{\partial \mu}{\partial T}) \) term in the numerator of Seebeck coefficient (see Eq. (16)), whereas the position of the peak depends on the ratio of \( L_\zeta^{(1)} \) and \( L_\zeta^{(1)} \). There is a change in sign of \( S \) while change in sign of \( \mu \) (due to \( (\epsilon - \mu) \) term in the numerator of \( S \)). It indicates the change in electrical nature of the charge carriers as \( \mu \) changes sign. When \( \mu \) lies in the conductance band, thermally activated electrons propagate opposite to the temperature gradient, which results in negative thermopower. On the other hand, when \( \mu \) lies in the valence band, thermally activated holes flow along the temperature gradient which leads to the positive thermopower. Similar to the conductance, the electron-hole symmetry is nearly perfect in this case (considering magnitude only) as well.

(b) Dependence on gap parameter: The figure reveals that the thermopower gets enhanced with increase in \( \eta \). From the the definition of Seebeck coefficient \( (S_\zeta \sim \frac{L_\zeta^{(1)}}{L_\zeta^{(0)}} \sim \frac{L_\zeta^{(1)}}{G_\zeta}) \), it is clear that an increase in \( L_\zeta^{(1)} \) and decrease in \( G_\zeta \) with \( \eta \) aid to enhance the value of the thermopower. Since \( L_\zeta^{(1)} \) increases and \( G_+ \) decreases with \( \eta \), \( S_+ \) starts to gain weight as we increase \( \eta \). On the other hand, \( G_- \) initially increases and \( L_\zeta^{(1)} \) decreases with \( \eta \) (as the gap decreases with \( \eta \) for \( \eta < 1 \)). For \( \eta = 1 \) (the gap vanishes), \( G_- \) and \( L_\zeta^{(1)} \) attain their maximum and minimum values respectively. For \( \eta > 1 \), \( G_- \) starts decreasing and \( L_\zeta^{(1)} \) starts increasing with \( \eta \). As a result, \( S_- \) initially decreases with \( \eta \), attains minimum value at \( \eta = 1 \) and then starts to increases as we increase \( \eta \). Though \( S_+ \) and \( S_- \) show different nature of variation with \( \eta \), the trend of variation of the charge Seebeck coefficient (for electrical conductance as well except the low chemical potential regime) as a function of \( \eta \) is similar to that of \( K \) valley (see Fig. (9)). This happens because \( K \) valley’s contribution in thermopower changes more rapidly with \( \eta \) as compared to \( K' \) valley. The reason behind this can be understood from Fig. (7), as it reveals that with increasing \( \eta \) from 0.5 to 2.0, the rate of change in \( T(\epsilon) \) in \( K \) valley is more than that in \( K' \) valley. As expected, the valley thermopower is smaller than the charge thermopower. Here, it should be noted that our system produces maximum thermopower, \( S_{\eta_{\text{max}}} = 3(k_B/e) \sim 258 \mu V/K \) (for \( \eta = 1.5 \)), whereas any
general graphene sheet can produce $\sim 50 - 100 \, \mu V/K$. It seems that on increasing the strength of $\eta$ even more, one can achieve higher thermopower. But it is not possible, as for such a higher value of $\eta$, there will be no available channel to conduct for the low chemical potential regime.

(c) **Dependence on tilt parameter**: It is worth mentioning that both the charge and valley polarized thermopower decrease with $v_t$. Though $v_t$ diminishes the conductance (the denominator of Seebeck coefficient), it lowers $T^{(1)}_c$ (numerator of $S_c$) too. Hence, the contribution of $(\frac{T^{(1)}_c}{\sigma_c} \pm \frac{T^{(1)}_v}{\sigma_v})$ (see the definition of charge and valley polarized Seebeck coefficient) decreases as we increase $v_t$.

The materials with large electron-hole asymmetry are known to enhance the thermoelectric coefficient. So more thermopower is expected when the middle region is made of tilted Dirac material instead of graphene. However, $v_t$ does not break the electron-hole symmetric nature in $T_c(\epsilon)$ as shown in Fig. (7)). Hence, it cannot aid to enhance the thermopower of the system. It is to be noted that if the middle region is also graphene (no tilt parameter), then for higher value of $\eta$, we don’t get any thermopower for the low chemical potential regime (around zero), whereas if the middle region is borophene or quinoid graphene we get finite values of thermopower for those low values of chemical potential. The physics behind this as follows – for graphene, in case of $\epsilon < |\Delta_c|$, there is no transmission because of imaginary momentum, and thus no channel to conduct. But for borophene or quinoid graphene, due to the indirect gap for the tilted velocity term, the momentum is real until $\epsilon > |\gamma_c/2|$, and hence few channels are available to conduct, although $\epsilon < |\Delta_c|$ (See Eq. (5) and Fig. (2)). Thus for low chemical potential, the highly gapped graphene-borophene-graphene junction is good candidate with respect to highly gapped graphene-graphene-graphene junction as a thermoelectric device.

### C. THERMAL CONDUCTANCE

(a) **Dependence on chemical potential**: In Fig. (10), we show the thermal charge conductance and valley polarized thermal conductance as a function of $\mu$. As $k_c$ arises due to the energy flow carried by the charge carriers, the thermal conductance as a function of $\mu$ show almost similar features as electrical conductance excepting the region where chemical potential is close to zero. In case of thermal conductance (see Fig. (10b)) there is a bump near $\mu = 0$, while for electrical charge conductance there is no such thing. This bump in thermal conductance arises due to the $(k_c)^{\text{el}}$ term shown in the inset of Fig. (10).

(b) **Dependence on gap parameter**: As expected, electrical thermal conductance shows the same nature as the electrical charge conductance as a function of $\eta$, which is depicted in Fig. (10). The reason behind this nature is same as for the charge conductance.

(c) **Dependence on tilt parameter**: Not surprisingly, the electrical thermal conductance as a function of $v_t$ shows the similar behavior as electrical charge conductance, that means the electrical thermal conductance is diminished by $v_t$. The above results and discussions on the electrical conductance, Seebeck coefficient and the thermal conductance will be helpful to understand the behavior of the figure of merit which we are going to discuss in the next section. Here we would like to mention that in our system, the Wiedmann-Franz law that states $\sigma_c/\kappa_c = L T$, where $L = 2.44 \times 10^{-8} \, \text{W} \cdot \text{Ω}^{-1} \cdot \text{K}^{-1}$ is the Lorentz number, $\sigma_c$ is electrical charge conductivity and $\kappa_c$ is the electrical thermal conductivity, holds for low temperature, though it deviates near $\mu = 0$. This law is valid in case of valley polarized conductivity as well under the same conditions.
D. FIGURE OF MERIT

(a) Dependence on chemical potential: The results of the thermoelectric figure of merit $ZT$ are shown in Fig. 11. The figure of merit mainly varies as $ZT \sim S^2$ which is depicted in Fig. 11. $ZT$ reaches its maximum value near $\mu \sim \pm 0.06$ eV, which is almost insensitive to $\eta$.

(b) Dependence on gap parameter: Figure 12 reveals that $\eta$ enhances both the charge and valley figure of merit. Since both $G_c$ and $k^{el}_c$ behave in a similar fashion with the increasing strength of $\eta$, their ratio does not contribute much for enhancing the figure of merit. But the enhanced $S_v$ with increasing $\eta$ helps to increase $ZT_c$. In case of valley figure of merit, both the parameters in numerator, $S_v$ and $G_v$, increase with the increasing strength of $\eta$ while the denominator, i.e., the $k^{el}_c$ decreases (except the region where $\mu \rightarrow 0$). Thus we get enhanced valley figure of merit with increasing strength of $\eta$. It is worth mentioning that our system yields maximum $ZT \sim 2$ (it will be slightly less if we include the phonon’s thermal conductance), which signifies that it is quite good as a thermoelectric device, since in most of the literature the reported $ZT$ is less than 2 \cite{[55]} and highest yet reported is $2.6$ \cite{[57]}.

(c) Dependence on tilt parameter: Finally, we study the effects of tilt parameter $v_t$ on $ZT$ which is shown in Fig. 12. Figure 12 depicts that the tilt parameter diminishes both the charge and valley polarized figure of merit. This is attributed to the fact that increase in $v_t$ reduces the thermopower (as discussed earlier) while the ratio of electrical and thermal conductance does not vary appreciably with $v_t$.

IV. CONCLUSION

We have studied the valley caloritronics of a photo-driven graphene/gapped tilted Dirac material/graphene junction and compared the results with the corresponding charge caloritronics. In particular, we have investigated the role of interplay among the valley index $\zeta$, tunable gap parameter $\eta = M/\Delta$ and the tilt parameter $v_t$ in the electrical conductance, thermal conductance, Seebeck coefficient and figure of merit of the junction device.

The band gaps in the tilted Dirac material become indirect in both the valleys due to tilt in the dispersion. The gaps at the two valleys are rendered unequal by the sum of Semenoff mass $M$ and photoinduced mass $\zeta \Delta$, where $\Delta$ may be varied by tuning the intensity of light. We have found that for $K$ valley, $\eta$ diminishes the charge conductance, whereas for $K'$ valley, it initially increases with $\eta$, attains maximum value at $\eta = 1$ and then decreases with $\eta$ when $\eta > 1$. This is attributed to distinctive nature of variation of $\Delta c$ in the two valleys with $\eta$. Furthermore, the total charge conductance $G_c$ coming from the two valleys decreases with $\eta$, whereas the valley polarized charge conductance $G_v$ shows the reverse trend. As a function of chemical potential ($\mu$), $G_c$ increases monotonically with $|\mu|$, while $G_v$ attains a peak and then asymptotically vanishes at higher values of $|\mu|$.

The electrical thermal conductance $\kappa$ as a function of $\eta$ and $\mu$ shows almost similar behavior as charge conductance, as it proportional to the amount of heat energy carried by the charge carriers. The variation of Seebeck coefficient $S_c$ (thermopower) as a function of $\eta$ is opposite to that of the $G_c$, as $S_c$ is inversely proportional to $G_c$. It implies that for $K$ valley, $\eta$ enhances the S while for $K'$ valley, S shows minimum value when $\eta = 1$. Both the total Seebeck coefficient, $S_c$ and valley polarized Seebeck coefficient, $S_v$ increase with $\eta$. The maximum absolute values of $S_c$ and $S_v$ is obtained at $\mu = \pm 0.04$ eV, which is roughly independent of $\eta$.

Since the ratio of $G$ and $\kappa$ does not show any significant change with $\eta$, the figure of merit as a function of $\eta$ shows a variation similar to square of Seebeck coeffi-
cient and its maximum value is obtained at $\mu = \pm 0.06$ eV. Furthermore, the tilt parameter reduces the effective transmission through the junction, thereby diminishing all the charge and valley polarized quantities. Finally, it can be concluded that owing to the tunability of $\eta$ by adjusting experimental setup, the fabrication of tunable thermoelectric device is achievable.

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Appendix A: Floquet Hamiltonian of a tilted Dirac material subjected to circularly polarized radiation

The Hamiltonian for quasiparticles with massive tilted anisotropic Dirac dispersion in the vicinity of two independent Dirac points in materials like borophene is given by [26-28]

$$H_B(q) = \zeta [v_x \sigma_x q_x + \zeta v_y \sigma_y q_y + v_0 \sigma_0 q_y] + M \sigma_z,$$  \hspace{1cm} (A1)

where $\sigma_x, \sigma_y$ are the Pauli matrices, $\sigma_0$ is the 2 $\times$ 2 identity matrix and $\zeta = \pm$ denotes the two independent Dirac points. $M \sigma_z$ is the mass term due to different onsite energies ($\pm M$) of the two sublattices. The energy dispersion and the corresponding wave functions associated with the Hamiltonian in Eq. (A1) are given by

$$E_{\lambda, \zeta}(q) = \hbar \zeta v_t q \sin \theta + \lambda \sqrt{M^2 + [\hbar q \Lambda(\theta)]^2}$$  \hspace{1cm} (A2)

and

$$\Psi^\lambda_{B}(r) = \frac{e^{iq \cdot r}}{\sqrt{2}} \left( \frac{1}{M + \lambda \sqrt{M^2 + [\hbar q \Lambda(\theta)]^2}} \right)^{1/2},$$  \hspace{1cm} (A3)

where $\delta = \tan^{-1}[v_y q_z/(v_x q_y)], \theta = \tan^{-1}(q_y/q_x)$ and $\Lambda(\theta) = \sqrt{(v_x \cos \theta)^2 + (v_y \sin \theta)^2}$ and $\lambda = \pm$ denotes the conduction and valence bands, respectively. Note that $v_t \neq 0$ term tilts the Dirac spectrum and is responsible for the electron-hole symmetry breaking, even for $v_x = v_y$ case.

Considering the borophene sheet is illuminated normally by intense circularly polarized electromagnetic radiation. The vector potential corresponding to the circularly polarized radiation is given by $A(t) = A_0 (\sin \omega t + j \cos \omega t)$, where $A_0 = E_0/\omega$ with $E_0$ being the amplitude of the electric field vector and $\omega$ is the frequency of the radiation. The vector potential is time-periodic since $A(t + T_\omega) = A(t)$, with the time-period $T_\omega = 2\pi/\omega$.

The time-periodic Hamiltonian in presence of the electromagnetic radiation is given by

$$H_B(q, t) = \zeta \hbar [v_x \sigma_x Q_x(t) + \zeta v_y \sigma_y Q_y(t) + v_0 \sigma_0 Q_y(t)] + M \sigma_z,$$  \hspace{1cm} (A4)

where $Q_i = q_i + eA_i(t)/\hbar$ with $i = x, y$. It is known that a gap in the Dirac spectrum can be induced in graphene, on the surface states of topological insulator, silicene, semi-Dirac systems, MoS$_2$ etc by off-resonant radiation. The off-resonant condition is achieved when the photon energy ($h \omega$) is much higher than the band width ($6\tau$ $\tau$ being the nearest-neighbor hopping energy) of the undriven borophene. In the off-resonant condition, the band structure is modified by the second-order virtual photon absorption-emission processes. The effective time-independent Floquet Hamiltonian in the off-resonant limit can be expressed as [58-60]

$$H_F(q) \simeq H_B(q) + \frac{[H_{-1}(q), H_{+1}(q)]}{\hbar \omega},$$  \hspace{1cm} (A5)

where the terms in the commutator are the Fourier components of $H(q, t)$,

$$H_{\pm 1}(q) = \frac{1}{T \omega} \int_0^{T \omega} dt e^{\pm i \omega t} H(q, t).$$  \hspace{1cm} (A6)

Using Eq. (A6) we find the commutator $[H_{-1}, H_{+1}]$ as given below,

$$\frac{[H_{-1}(q), H_{+1}(q)]}{\hbar \omega} = \frac{\zeta e^2 A_0^2 v_x v_y}{\hbar \omega} \sigma_z = \zeta \Delta \sigma_z,$$  \hspace{1cm} (A7)

where $\Delta = (eA_0)^2 v_x v_y/\hbar \omega$ is the gap at the Dirac points, an experimentally tunable parameter. The gap parameter $\Delta$ does not depend on the tilt parameter $v_t$.

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