Optimal band gap for improved thermoelectric performance of two-dimensional Dirac materials

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Thermoelectric properties of two-dimensional (2D) Dirac materials are calculated within linearized Boltzmann transport theory and relaxation time approximation. We find that the gapless 2D Dirac material exhibits poorer thermoelectric performance than the gapped one. Furthermore, there exists an optimal band gap for maximizing figure of merit (ZT) in the gapped 2D Dirac material. The optimal band gap ranges from $6k_B T$ to $18k_B T$, where $k_B$ is the Boltzmann constant and $T$ is the operating temperature in kelvin. This result, which is similar to that for bulk semiconductors, indicates the importance of having narrow gaps to achieve the best thermoelectrics in 2D systems. Larger maximum ZTs can also be obtained by suppressing the lattice thermal conductivity. In the most ideal case where the lattice thermal conductivity is zero (leaving the electron thermal conductivity alone), the maximum ZT in the gapped 2D Dirac material is many times ZT of commercial thermoelectric materials.

I. INTRODUCTION

Thermoelectric (TE) materials convert temperature gradient into electricity and thus they are useful for various devices utilizing refrigerators and power generators [1,2]. However, it is also well recognized that the efficiency of most of TE materials is lower than other energy conversion systems so their applications are still limited in the areas where the efficiency is not an important issue. To expand the applicability of thermoelectrics, there has been extensive studies suggesting different strategies with particular emphasis on improving the efficiency, such as the energy band convergence [3], the hierarchical archi- tecturing [4], and the low-dimensional materials [5, 6]. Theoretically, an efficient TE material should be a good electronic conductor as well as a good thermal insulator. The efficiency of converting heat into electricity is related to the so-called TE figure of merit, $ZT = S^2 \sigma T/\kappa$, where $S$, $\sigma$, $\kappa$, and $T$ are the Seebeck coefficient, electrical conductivity, thermal conductivity, and operating temperature, respectively. For many decades, it has been a challenging issue even just to find materials with $ZT \approx 1$ since $S$, $\sigma$, and $\kappa$ are generally interrelated [7, 8]. In other words, it is difficult to obtain a TE material with simultaneously large $S$, large $\sigma$, and small $\kappa$ to maximize $ZT$ [9, 10].

Of different strategies to obtain better $ZT$, miniaturization of materials has been an important route to enhance TE performance, thanks to the quantum confinement effect that modifies the band structure, effective mass, and density of states [5, 6, 12, 13]. Two-dimensional (2D) materials, in particular, are often suggested to have better TE performance than bulk materials [14, 15]. For example, a large power factor, $S^2 \sigma$ (part of the numerator of $ZT$), has been either theoretically proposed or experimentally observed in various classes of 2D materials such as MoS$_2$ [16], SnS$_2$ [17], InSe [18], and some graphene-like materials [19]. Furthermore, by band gap engineering, these 2D materials possess various values of the band gaps, ranging from nearly zero to about 2 eV [20–23], so we may have a lot of choices of materials depending on the purpose. However, the $ZT$ of 2D materials overall remains hard to push above unity. In particular, for the 2D materials with moderate or wide band gaps, the predicted or observed $ZT$ values are mostly less than one [16–18], while the 2D materials with smaller gaps tend to exhibit larger $ZT$ [24]. This tendency reminds us to some of the early works regarding the effect of band gap on the $ZT$ [9, 10], in which it was suggested that the best thermoelectrics in bulk (3D) systems can be obtained with materials having narrow gaps [11, 25]. Motivated by those works, we are wondering if there also exists an optimal gap (or a possible range of optimal gaps) for the 2D materials in order to achieve the best thermoelectrics, which can guide experimentalists to search for 2D materials with high TE performance.

In this work, we focus our attention to the 2D materials whose electronic structure can be modeled by the Dirac Hamiltonian, or the so-called 2D Dirac materials. In fact, most of monolayer 2D materials having excellent electron transport properties can be considered as the 2D Dirac materials, thanks to presence of nonparabolic bands with linear energy dispersion around the Dirac point for the gapless case. As we will show later, the excellent electron transport properties in these materials do not automatically lead to efficient and high-performance thermoelectrics. However, we can maximize the $ZT$ for the 2D Dirac materials by considering the optimal gap. From the calculations of the Seebeck coefficient, electrical con-
ductivity, thermal conductivity, and thus $ZT$ within linearized Boltzmann transport theory and relaxation time approximation (RTA), we find that the optimal gaps for the 2D Dirac materials are about $6–18k_BT$. This result is similar with the case of bulk semiconductors whose optimal gaps for the maximal $ZT$ are about $6–10k_BT$ (the upper limit may be larger depending on the dominant scattering mechanism) [11]. Therefore, although recent trend in TE research utilize moderate-gap or wide-gap 2D semiconductors as potential TE materials [16–18], we would suggest that it is better to use materials with narrow band gaps within $6–18k_BT$ and then, if needed, we may further enhance their TE performance by other techniques such as doping [26], strain engineering [27], and manufacturing grain boundary or point defect [28] to diminish the phonon thermal conductivity.

II. MODEL AND METHODS

For simplicity, we assume that the energy bands of gapless and gapped Dirac materials are symmetric with respect to $E = 0$. The 2D Dirac material with a band gap $E_g = 2\Delta$ can be described by energy dispersion,

$$E(k) = \pm \sqrt{\hbar^2 |k|^2 + \Delta^2}, \quad (1)$$

where $\hbar$ is the Planck constant, $v_g$ is the group velocity, and $k$ is the 2D wave vector with magnitude $k = |k| = \sqrt{k_x^2 + k_y^2}$. This energy dispersion is illustrated in Figs. 1(a) and (b) for gapless ($\Delta = 0$) and gapped (finite $\Delta$) 2D Dirac materials, respectively.

We use the Boltzmann transport theory in the linear response regime and apply the relaxation time approximation (RTA) for an isotropic system, which is valid for our simplified model of 2D Dirac materials whose transport properties do not depend on a particular orientation in the 2D plane. Within this approach, thermoelectric properties of a 2D Dirac material with electronic energy dispersion can be calculated from the transport coefficients

$$L_i = \int_{-\infty}^{\infty} T(E)(E - \mu)^i \left(-\frac{\partial f}{\partial E}\right) dE, \quad (2)$$

where $\mu$ is the chemical potential (or Fermi energy), $f(E)$ is the Fermi-Dirac distribution, and $T(E)$ is the transport distribution function (TDF). In Eq. (2), $i$ takes a value of 0, 1, or 2 depending on the thermoelectric properties to be calculated.

The explicit form of TDF is

$$T(E) = v^2(E)\tau(E)D(E), \quad (3)$$

where $v$ is the longitudinal velocity in a particular direction, $\tau$ is the relaxation time, and $D(E)$ is the density of states (DOS). Due to the isotropic nature of the 2D Dirac materials in our model, $v$ can be related with $v_g$ by the following formula:

$$v^2 = \frac{v_g^2}{2} \left(\frac{E^2 - \Delta^2}{E^2}\right). \quad (4)$$

For the energy-dependent relaxation time, we assume that short-ranged impurity scattering dominates the relaxation mechanism and as result the relaxation time is inversely proportional to the DOS [29, 30], i.e.,

$$\tau(E) = C [D(E)]^{-1}, \quad (5)$$

where $C$ is the scattering coefficient in units of $W^{-1}m^{-3}$. This assumption can be derived from Fermi’s golden rule and is suitable for the scattering mechanism involving electron-phonon interactions where either acoustic or optical phonons scattered by electrons within temperature range 300–700 K [29, 31]. For the sake of completeness, in Appendix we also present the calculation result within a less accurate assumption of constant $\tau$ (relaxation time independent of $E$), which is still widely used in the literature [32].

Using the transport coefficients, one can calculate the electrical conductivity $\sigma$, Seebeck coefficient $S$, and electron thermal conductivity $\kappa_e$. They are respectively given by

$$\sigma = q^2L_0, \quad (6)$$
$$S = \frac{1}{qT}L_1, \quad (7)$$

and

$$\kappa_e = \frac{1}{T} \left( L_2 - \frac{(L_1)^2}{L_0} \right). \quad (8)$$

From these thermoelectric properties, along with the lattice thermal conductivity $\kappa_{ph}$, we can calculate the thermoelectric figure of merit,

$$ZT = \frac{S^2\sigma}{\kappa_e + \kappa_{ph}}T. \quad (9)$$

Whenever necessary, especially to simplify some equations, we will use reduced (dimensionless) variables for the energy dispersion $\varepsilon = E/k_BT$, and also for the chemical potential, $\eta = \mu/k_BT$.

The transport coefficients $L_i$ are generally calculated by considering all bands available within $E = (-\infty, \infty)$. However, in most of materials, thermoelectric properties are dominated by the states near the Fermi energy. In this work, we adopt the two-band model involving a valence band and a conduction band as a minimum requirement to include the bipolar effect (or sign inversion of the Seebeck coefficient), which is always observed in materials having two different types of carriers, i.e., electrons...
and holes in the conduction and valence bands, respectively. In the two-band model, \( \sigma, S, \) and \( \kappa_e \) can be written as follows \( ^{11} \):

\[
\sigma = \sigma_c + \sigma_v, \tag{10}
\]

\[
S = \frac{\sigma_c S_c + \sigma_v S_v}{\sigma_c + \sigma_v}, \tag{11}
\]

\[
\kappa_e = \frac{\sigma_c \sigma_v}{\sigma_c + \sigma_v} (S_c - S_v)^2 + (\kappa_{e,c} + \kappa_{e,v}), \tag{12}
\]

where the additional subscript \( c \) (\( v \)) labels the conduction (valence) band.

Based on Eqs. (10)–(12), the integral \( \mathcal{L}_i \) in Eqs. (6)–(8) can be decomposed into \( \mathcal{L}_{i,c} \) and \( \mathcal{L}_{i,v} \) with the integration over energy intervals \( [0, \infty) \) and \( \left( -\infty, 0 \right] \) for the valence and conduction bands, respectively, i.e.,

\[
\mathcal{L}_{i,c} = \int_0^\infty T(E)(E - \mu)^i \left( -\frac{\partial f}{\partial E} \right) dE. \tag{13}
\]

and

\[
\mathcal{L}_{i,v} = \int_{-\infty}^0 T(E)(E - \mu)^i \left( -\frac{\partial f}{\partial E} \right) dE. \tag{14}
\]

We will show detailed calculations of \( \mathcal{L}_{i,c} \) and \( \mathcal{L}_{i,v} \) for the gapless 2D Dirac material in Sec. III because it is possible to analytically obtain these integrals for the gapless case. Some variable and unit notations introduced in Sec. III will also be later used in Secs. IV and V when discussing more general cases (both gapped and gapless 2D Dirac materials), in which it is necessary to perform the integration numerically.

### III. GAPLESS 2D DIRAC MATERIAL

In the gapless 2D Dirac material, \( \Delta = 0 \) leads to the TDF independent of \( E \) because the group velocity \( v_g \) of the massless Dirac electron is constant, \( T = v_g^2 C/2 \).

To calculate the integral \( \mathcal{L}_i \), we can separate the energy interval \( [0, \infty) \) for the conduction band and \( \left( -\infty, 0 \right] \) for the valence band. For the conduction band, we obtain \( \mathcal{L}_i \) as

\[
\mathcal{L}_{i,c} = \frac{1}{2} v_g^2 C(k_B T)^i \mathcal{F}_{i,c}(\eta), \tag{15}
\]

with

\[
\mathcal{F}_{i,c}(\eta) = \int_{-\eta}^{\infty} x^i e^x (e^x + 1)^2 dx \tag{16}
\]

due to the substitution of \( x = \varepsilon - \eta \). For \( i = 0, 1, 2 \), we have:

\[
\mathcal{F}_{0,c}(\eta) = \frac{e^\eta}{e^\eta + 1}, \tag{17}
\]

\[
\mathcal{F}_{1,c}(\eta) = \frac{\eta}{e^\eta + 1} + \ln(1 + e^{-\eta}), \tag{18}
\]

\[
\mathcal{F}_{2,c}(\eta) = \frac{\pi^2}{3} - \frac{\eta^2}{e^\eta + 1} - 2\eta \ln(1 + e^{-\eta}) + 2L_2(-e^{-\eta}), \tag{19}
\]

where \( L_j(z) = \sum_{n=1}^\infty \frac{z^n}{n^j} \) is the polylogarithmic function.

We obtain \( \sigma_c, S_c, \) and \( \kappa_{e,c} \) as follows:

\[
\sigma_c = q^2 \mathcal{L}_{0,c} = \frac{1}{2} e^2 g^2 C \mathcal{F}_{0,c}(\eta), \tag{20}
\]

\[
S_c = \frac{1}{qT \mathcal{L}_{0,c}} \mathcal{L}_{1,c} = \frac{k_B \mathcal{F}_{1,c}(\eta)}{e \mathcal{F}_{0,c}(\eta)}, \tag{21}
\]

\[
\kappa_{e,c} = \frac{1}{T} \left( \mathcal{L}_{2,c} - \left( \frac{\mathcal{L}_{1,c}}{\mathcal{L}_{0,c}} \right)^2 \right) = \frac{1}{2} v_g^2 C k_B T \left( \mathcal{F}_{2,c}(\eta) - \left( \frac{\mathcal{F}_{1,c}(\eta)}{\mathcal{F}_{0,c}(\eta)} \right)^2 \right), \tag{22}
\]

where \( e \approx 1.602 \times 10^{-19} \text{ C} \) is the elementary charge. For convenience, hereafter we will use the units \( S_0 = k_B/e \) (\( \sim 87 \) \( \mu \text{V/K} \)), \( \sigma_0 = e^2 g^2 C/2 \), and \( \kappa_0 = v_g^2 C k_B T/2 \). We also set the lattice thermal conductivity as an adjustable quantity,

\[
\kappa_{ph} = r_K \kappa_0, \tag{23}
\]

where \( r_K \) is a material parameter and may be engineered to maximize the \( ZT \).

Considering only the conduction band, the figure of merit for the gapless 2D Dirac material is given by:

\[
ZT_c(\eta) = \frac{S_c^2 \sigma_c}{\kappa_{e,c} + \kappa_{ph}} T = \frac{(\mathcal{F}_{1,c}(\eta))^2}{\mathcal{F}_{0,c}(\eta) \mathcal{F}_{2,c}(\eta) - (\mathcal{F}_{1,c}(\eta))^2 + r_K \mathcal{F}_{0,c}}, \tag{24}
\]
Although $ZT$ may have a finite value if we only consider the conduction band as represented by $ZT_c$, the full expression of the two-band model gives additional terms related to the valence band that will cancel $ZT_c$ and lead to $ZT = 0$ for the gapless 2D Dirac material as shown below.

The TE integral $\mathcal{L}_i$ for the valence band is

$$\mathcal{L}_{i,v} = \frac{1}{2} v_g^2 C (k_B T)^4 F_{i,v}(\eta),$$

with

$$F_{i,v}(\eta) = \int_{-\infty}^{-\eta} \frac{x^2 e^x}{(e^x + 1)^3} dx.$$  \hspace{1cm} (26)

For $i = 0, 1, 2$, we have:

$$F_{0,v}(\eta) = \frac{1}{e^\eta + 1},$$

$$F_{1,v}(\eta) = -\frac{\eta}{e^\eta + 1} - \ln(1 + e^{-\eta}),$$

$$F_{2,v}(\eta) = \frac{\eta^2}{e^\eta + 1} + 2x \ln(1 + e^{-\eta}) - 2 \text{Li}_2(-e^{-\eta}).$$

Note that the integrals $\mathcal{F}_{i,c}$ and $\mathcal{F}_{i,v}$ are connected via electron-hole symmetry of the system:

$$\mathcal{F}_{0,c}(\eta) = \mathcal{F}_{0,v}(-\eta),$$

$$\mathcal{F}_{1,c}(\eta) = -\mathcal{F}_{1,v}(\eta),$$

$$\mathcal{F}_{2,c}(\eta) = \mathcal{F}_{2,v}(-\eta).$$

The contribution of the valence band to the thermoelectric quantities $\sigma_v$, $S_v$, and $\kappa_{v,e}$, can be expressed similarly with that of the conduction band:

$$\sigma_v = \sigma_0 F_{0,v}(\eta),$$

$$S_v = -S_0 \frac{F_{1,v}(\eta)}{F_{0,v}(\eta)},$$

$$\kappa_{e,v} = \kappa_0 \left( \frac{F_{2,v}(\eta)}{F_{0,v}(\eta)} - \frac{(F_{1,v}(\eta))^2}{F_{0,v}(\eta)} \right).$$

Based on the formulas of the two-band model [Eqs. (10)–(12)] and the electron-hole symmetry in the TE integrals [Eq. (30)], it is obvious that the Seebeck coefficient $S$ becomes zero [see Fig. 2(a)], whereas the electrical conductivity $\sigma$ and electron thermal conductivity $\kappa_e$ have nonzero (finite) values that are constant for whole $\eta$ [see Figs. 2(b) and (c)]. As a result, for the gapless 2D Dirac material considered in this work, we have

$$ZT(\eta) = 0.$$  \hspace{1cm} (34)

This dramatic result underscores the demerit of electron-hole symmetry for TE performance [see dotted and dashed lines in Figs. 2(a)–(c)]. The competing contribution of electrons and holes persists in the electron-hole symmetric band structures even when the energy gap is introduced. Since the relaxation time is assumed to be inversely proportional to DOS in Eq. (14), the TDF becomes energy-independent and the Seebeck coefficient completely vanishes for all doping levels. We note that such a model fails to describe the region near the Dirac point ($\mu = 0$) as the DOS vanishes. In the realistic situation, the accidentally perfect cancellation may not appear due to the complexity of the scattering mechanism and imperfect electron-hole symmetry. For example, finite Seebeck’s coefficient $S \approx 40 – 100$ $\mu$V/K at 300 K was reported for the 2D graphene [33, 34].

The finite Seebeck coefficient is thus expected with dominant contribution coming from the majority carrier (either electron or hole depending on the sign of chemical potential). Although qualitatively less accurate from our theoretical point of view, the constant $\tau$ approximation presented in Appendix gives nonzero and finite value of $S$ for the gapless 2D Dirac material. Sharapov and Varlamov in an earlier work also predicted within the constant $\tau$ approximation the nonzero value of $S$ in gapless graphene and anomalous growth of $S$ in gapped graphene [35]. To get rid of the poor TE performance due to the electron-hole cancellation, we may apply a magnetic field as a facilitator to break the electron-hole symmetry and thus obtain a larger, nonsaturating Seebeck coefficient [36]. However, applying the magnetic field on the order of several teslas is beyond the current practical capability of the TE industry.
IV. GAPPED 2D DIRAC MATERIAL

Unlike for the gapless 2D Dirac material, the TDF for the gapped 2D Dirac material is now energy-dependent:

\[ T(E) = \frac{C e^2 g}{2} \left( \frac{E^2 - \Delta^2}{E^2} \right), \quad (35) \]

with the energy intervals \([-\infty, -\Delta]\) and \([\Delta, \infty]\) to be considered in the calculation of the TE integrals. For simplifying the formulation, we define the dimensionless gap,

\[ \tilde{\Delta} = \Delta/k_B T \quad (36) \]

The TE integral for the conduction band is

\[ \mathcal{L}_{i,c} = \frac{C e^2 g (k_B T)^i}{2} \left( \mathcal{F}_{i,c}(\eta) - \mathcal{G}_{i,c}(\tilde{\Delta}, \eta) \right), \quad (37) \]

with

\[ \mathcal{G}_{i,c}(\tilde{\Delta}, \eta) = \int_{-\tilde{\Delta}}^{\tilde{\Delta}} \frac{\tilde{\Delta}^2}{(x + \eta)^2 (e^x + 1)^2} dx. \quad (38) \]

Similarly, the TE integral for the valence band is

\[ \mathcal{L}_{i,v} = \frac{C e^2 g (k_B T)^i}{2} \left( \mathcal{F}_{i,v}(\eta) - \mathcal{G}_{i,v}(\tilde{\Delta}, \eta) \right), \quad (39) \]

with

\[ \mathcal{G}_{i,v}(\tilde{\Delta}, \eta) = \int_{-\tilde{\Delta}}^{-\eta} \frac{\tilde{\Delta}^2}{(x + \eta)^2 (e^x + 1)^2} dx. \quad (40) \]

The \( \mathcal{G}_i \) integrals for the conduction and valence band contributions are calculated numerically.

Figure 3 depicts the TE properties of the 2D gapped Dirac material. The calculation result of Seebeck coefficient shows finite values which sign changes across the charge neutrality point, indicating competing contribution of electron and hole, as represented by dotted and dashed lines in Fig. 3(a). The electrical conductivity exhibits a dip in the band gap and saturates to a finite value far away from the gap [Fig. 3(b)]. On the other hand, electron thermal conductivity shows a local maximum at the gap due to the combination of \( S_{e,v} \) and \( \kappa_{e,v} \) that add each other. The resulting \( ZT \) peaks appear slightly above the band edges with a maximum value of about 0.2 for \( \tilde{\Delta} = 1 \) if no phonon contributes to the thermal conductivity \( (r_\kappa = 0) \). The \( ZT \) peaks monotonically decrease as the phonon contribution to the thermal conductivity increases.

V. OPTIMAL BAND GAP FOR BETTER THERMOELECTRICS

Understanding how band gap alters the TE properties is of importance for designers of TE materials. To see the evolution of TE properties with respect to the band gap, we show in Fig. 4 the calculation results of \( S, \sigma, \kappa_e, \) and \( ZT \) for \( \Delta = 0 \)– 8. As the band gap increases, the Seebeck coefficient monotonically decreases while electrical and electron thermal conductivities increase. Combined action of these interrelated quantities shall give \( ZT \) that can be maximized by tuning \( \Delta \). For \( r_\kappa = 1 \), the \( ZT \) value reaches maximum near the band edge and becomes largest at \( \Delta = 4 \) or corresponding band gap \( E_g = 8k_B T \) [Fig. 4(d)].
To find the optimal band gap for the 2D Dirac materials, we can numerically calculate the maximum $ZT$ value scanned through doping levels $\mu$ and then plot $ZT_{\text{max}}$ (the maximum $ZT$ found after scanning $\mu$) as a function of $E_g$ and $r_k$. The result is shown in Fig. 5. We can see that $ZT_{\text{max}}$ typically peaks at $E_g \approx 6k_BT$ depending on phonon thermal conductivity coefficient $r_k$. By the increase of $r_k$, we find that $ZT_{\text{max}}$ tends to be achieved at smaller band gap, saturated at $E_g \sim 6k_BT$. Decreasing phonon thermal conductivity through different methods such as defect engineering, heterostructures and strain is favorable to enhance $ZT$. For example, the ultralow thermal conductivity denoted by $r_k = 0$ will give the largest possible $ZT_{\text{max}}$ far above unity and it favors larger band gap of about $18k_BT$ as shown in the inset of Fig. 5.

VI. CONCLUSIONS AND PERSPECTIVE

We have shown that optimal band gaps within 6–18$k_BT$ are useful for maximizing $ZT$ in the 2D Dirac materials, where the TE properties were calculated considering the energy-dependent relaxation time $\tau(E)$ inversely proportional to the DOS. This result indicates that the gapless 2D Dirac material is not good for thermoelectrics, but opening a gap of few $k_BT$ is beneficial to enhance its TE properties. The candidates of the gapped 2D Dirac materials that are suitable for TE applications may already possible to fabricate, such as bilayer graphene (with electrically tunable gap) and commensurate graphene-hBN heterostructure [34, 37] whose miniband about tens of meV emerges due to inversion symmetry breaking. In particular, the graphene-hBN heterostructure has excellent $S^2\sigma$ [34]. Next, reducing the phonon thermal conductivity to reach $ZT$ that are satisfactory for the TE applications is worth investigating. Our model is also readily extensible for other systems by using appropriate parameters, so that it may trigger further theoretical works on thermoelectrics. Multiband effect which is not considered in this calculation might enhance ZT and can be incorporated in a straight-forward fashion within linearized Boltzmann transport equation.

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Appendix: Results within constant relaxation time approximation (CRTA)

Here we present the calculation of TE properties of 2D Dirac materials within the constant relaxation time approximation (CRTA). The results within this approximation overestimate the value of $S$ and $\sigma$ in comparison to those given in the main text. As a result, the gapless 2D Dirac material will have finite (nonzero) $S$, unlike what we have shown in the main text.

In the CRTA, the transport distribution function for the 2D Dirac materials is given by

$$T(E) = \tau_0 \left[ \frac{v_F^2}{2} \left( \frac{E^2 - \Delta^2}{E^2} \right) \right] D(E),$$  \hspace{1cm} (A.1)

where $\tau_0$ is the relaxation time constant. The density of states is defined by

$$D(E) = \frac{g|E|}{2\pi L(\hbar v_F)^2} \Theta(|E| - |\Delta|),$$  \hspace{1cm} (A.2)

where $g$ is degeneracies, $L$ is the confinement length, and $\Theta(x)$ is the Heaviside step function, i.e., $\Theta(x) = 1$ if $x > 0$ and $\Theta(x) = 0$ otherwise.

After some algebra [32], we can obtain the TE integral for the conduction band of the 2D Dirac material within the CRTA as

$$\mathcal{L}_{i,c} = \frac{g\tau_0}{4\pi \hbar^2 L} (k_BT)^{i+1} \left[ \mathcal{F}_{i+1,c}(\eta - \tilde{\Delta}) + \eta \mathcal{F}_{i,c}(\eta - \tilde{\Delta}) - \tilde{g}_{i,c}(\tilde{\Delta}, \eta) \right],$$  \hspace{1cm} (A.3)

with

$$\tilde{g}_{i,c}(\tilde{\Delta}, \eta) = \int_{\tilde{\Delta} - \eta}^{\infty} \frac{\tilde{\Delta}^2}{(x + \eta)} \left( e^{x} + 1 \right)^2 dx.$$  \hspace{1cm} (A.4)

Similarly, the TE integral for the valence band is

$$\mathcal{L}_{i,v} = - \frac{g\tau_0}{4\pi \hbar^2 L} (k_BT)^{i+1} \left[ \mathcal{F}_{i+1,v}(\eta + \tilde{\Delta}) + \eta \mathcal{F}_{i,v}(\eta + \tilde{\Delta}) - \tilde{g}_{i,v}(\tilde{\Delta}, \eta) \right].$$  \hspace{1cm} (A.5)
FIG. 6. Thermoelectric properties of gapless 2D Dirac material as a function of chemical potential within the CRTA. (a) Seebeck coefficient in units of \( S_0 = k_B/e \). (b) Electrical conductivity in units of \( \sigma_0 = g_0 e^2 k_B T / (4\pi h^2 L) \). (c) Electron thermal conductivity in units of \( \kappa_0 = g_0 k_B T^2 / (4\pi h^2 L) \). (d) Dimensionless figure of merit calculated with three different parameters \( r_c \) (representing lattice thermal conductivity).

FIG. 7. Thermoelectric properties of a 2D Dirac material within the CRTA for \( \Delta = 1 \) (equivalently, band gap \( E_g = 2k_F T \)). (a) Seebeck coefficient in units of \( S_0 = k_B/e \). (b) Electrical conductivity in units of \( \sigma_0 = g_0 e^2 k_B T / (4\pi h^2 L) \). (c) Electron thermal conductivity in units of \( \kappa_0 = g_0 k_B T^2 / (4\pi h^2 L) \). (d) Dimensionless figure of merit calculated with three different parameters \( r_c \) (representing lattice thermal conductivity).

with

\[
\overline{\tau}_{i,v}(\Delta, \eta) = \int_{-\infty}^{-\Delta-\eta} \frac{\Delta^2}{(x + \eta)} \frac{x^2 e^x}{(e^x + 1)^2} dx. \tag{A.6}
\]

The remaining calculation procedure to obtain the TE properties is the same as in the main text. Due to the complexity of \( L_i \), the integration in this case should also be performed numerically.

Note that, in addition to \( F_0 \), \( F_1 \), and \( F_2 \), we have to employ \( F_3 \) according to the recursive relation of \( L_i \) in Eqs. (A.3) and (A.5). The formulas for \( F_{3,e} \) and \( F_{3,v} \) are

\[
F_{3,e}(\eta) = \eta^2 \left[ \frac{\eta}{1 + e^\eta} + 3 \ln (1 + e^{-\eta}) \right] - 6\eta \text{Li}_2(-e^{-\eta}) - 6 \text{Li}_3(-e^{-\eta}) \tag{A.7}
\]

and

\[
F_{3,v}(\eta) = \eta^2 \left[ -\frac{\eta}{1 + e^\eta} - 3 \ln(1 + e^{-\eta}) \right] + 6\eta \text{Li}_2(-e^{-\eta}) + 6 \text{Li}_3(-e^{-\eta}) \tag{A.8}
\]

respectively.

Figures 6 and 7 show the results of TE properties of the 2D Dirac materials within the CRTA by using the same parameters as in Figs. 2 (gapless, \( \Delta = 0 \)) and 3 (gapped, \( \Delta = 1 \)). Within the CRTA, we can see that all the TE properties are overestimated. The most notable feature is the nonzero \( S \) for the gapless 2D Dirac material [Fig. 6(a)], which leads to the finite \( ZT \) [Fig. 6(d)] for different \( r_c \) values. Similarly, \( ZT \) for the gapped 2D Dirac material within the CRTA is also larger than that shown in the main text.

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