

Berry-phase-mediated topological thermoelectric transport in gapped single and bilayer graphene

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We consider the anomalous thermoelectric transport in gapped single and bilayer graphene where the gap may be due to broken inversion symmetry. In the presence of the gap, nontrivial Berry phase effects can be shown to mediate a transverse thermoelectric voltage in response to an applied temperature gradient even in the absence of a perpendicular magnetic field. This spontaneous anomalous Nernst effect is nonzero for nonuniform chemical potential in the two inequivalent valleys in the graphene band structure. Conversely, the Nernst response can be used to create a valley-index polarization between the two transverse sample edges as in the analogous valley Hall effect.

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I. INTRODUCTION

Interesting electric transport properties of the Dirac quasiparticles of graphene have recently come under focus.¹⁻⁵ Graphene, which consists of a single layer of carbon atoms in a bipartite honeycomb lattice, has a unique band structure that includes two inequivalent valleys in the first Brillouin zone of the momentum space. In gapless graphene, the valleys are characterized by the conduction and the valence bands touching each other at zero energy. Near the valleys, the appropriate quasiparticle dispersion relations are linear in momentum, similar to those of massless Dirac quasiparticles. Intervalley scattering is generally suppressed⁶⁻⁸ and will be ignored here due to the absence of a large-enough scattering wave vector mixing the two Dirac points.

In some graphene samples, e.g., epitaxial graphene on SiC substrate, a sizable gap has been reported⁹ in the quasiparticle spectrum near the Dirac points. Since the gap approaches zero with increasing sample thickness, it has been attributed to the effects due to the substrate, which is believed to break the sublattice [hence, the space inversion (SI) symmetry].⁹ Note that a quasiparticle gap in graphene can also result from confined geometries such as in the graphene nanoribbons.^{10,11} In bilayer graphene, an applied interlayer voltage bias can lead to a gap due to broken SI symmetry.¹² In such systems, the effects of the momentum space Berry curvature,¹³ which is sharply peaked at the two valleys, give rise to nontrivial, topological, and electric transport phenomena.^{14,15} In this paper, we discuss the effects of the topological Berry phases on another class of transport coefficients, the thermoelectric response coefficients. We will focus, in particular, on the topological Nernst effect of gapped graphene. In light of the recent successful measurements of the regular thermoelectric coefficients in graphene,¹⁶⁻¹⁸ the anomalous topological Nernst response we discuss here acquires particular relevance and importance. Although the specific calculations in this paper apply to graphene samples with broken SI symmetry, they should, more generally, be qualitatively valid in the presence of a gap of any origin near the Dirac points. Note that an energy gap is ultimately essential for the use of graphene as an electronic material.

We calculate the Berry-phase-supported spontaneous (i.e., it exists even without an external magnetic field) Nernst effect of the low-energy quasiparticles in graphene and show that it is nonzero for a nonzero valley polarization in the sample. While a nonzero valley polarization can be artificially created,¹⁹ it can also be induced by an applied magnetic field itself in a generic Nernst measurement setup.¹⁵ The regular Nernst effect in gapped graphene may, therefore, have a substantial anomalous contribution because of the induced valley polarization. Even in the absence of any valley polarization, the spontaneous Nernst signals are nonzero from the individual valleys but are equal and opposite to each other so the total signal is zero. Therefore, they can be used to create a nonzero valley polarization on the transverse edges, which can be technologically important.

In recent experiments, thermoelectric coefficients, in particular, the Nernst coefficient, have been measured for nonzero transverse magnetic fields in gapless graphene.¹⁶⁻¹⁸ The topological Nernst effect we discuss here exists even in the absence of any external magnetic field; it is solely driven by the effective magnetic field, given by the Berry curvature, near the valley centers in the momentum space. In the thermoelectric experiments, a temperature gradient $-\nabla T$ applied along, say, the \hat{x} direction produces a measurable transverse electric field. The total charge current in the presence of the electric field \mathbf{E} and $-\nabla T$ is given by $J_i = \sigma_{ij} E_j + \alpha_{ij} (-\partial_j T)$, where σ_{ij} and α_{ij} are the electric and the thermoelectric conductivity tensors, respectively. Setting \mathbf{J} to zero, the Nernst signal, defined as $e_N \equiv E_y / |\nabla T| = \rho \alpha_{xy} - S_{xx} \tan \theta_H$, is measured, where α_{xy} is the Nernst conductivity defined via the relation $J_x = \alpha_{xy} (-\partial_y T)$ in the absence of the electric field, $\rho = 1 / \sigma_{xx}$ is the longitudinal resistance, $S_{xx} = E_x / |\nabla T| = \rho \alpha_{xx}$ is the thermopower, and $\tan \theta_H = \sigma_{xy} / \sigma_{xx}$ is the Hall angle. If the second term is small, which is sometimes the case,²⁰ $\rho \alpha_{xy}$ completely defines the Nernst signal, but in the most general case one should extract α_{xy} from the experimental data to compare with our calculations.

In this paper, the Berry-phase-mediated topological contribution to α_{xy} is calculated through two different approaches. In the first path-integral method, we first compute the frequency-dependent off-diagonal component of the elec-

tric conductivity tensor, $\sigma_{ij}(\Omega)$, for the Dirac quasiparticles in graphene. At low temperatures, the Nernst conductivity α_{xy} can be related to the zero temperature dc Hall conductivity σ_{xy} through the Mott relation²¹ [Eq. (22)]. This method has the advantage that it produces, as a by-product, the imaginary part of the ac Hall conductivity, σ_{xy}'' , which can be related to the possible polar Kerr effect^{22,23} in graphene. Indeed, in the case of a nonzero valley-index polarization in the sample, the Berry-phase-induced polar Kerr effect will be nonzero and observable. Another advantage of this method is that it can give a neat analytical expression of the Nernst conductivity at low temperatures. The effects of quasiparticle nonlinear dispersion relations on the topological transport properties of graphene have also been discussed in this framework. This method, however, is approximate and gives the values of the Nernst coefficient only at low-enough temperatures. In a more general method, which is valid also at higher temperatures, the anomalous contribution to α_{xy} can be calculated from the coefficient $\bar{\alpha}_{xy}$, which determines the transverse heat current \mathbf{J}^h in response to an electric field \mathbf{E} : $J_x^h = \bar{\alpha}_{xy} E_y$. The coefficients are related to one of the Onsager relations: $\bar{\alpha}_{xy} = T\alpha_{xy}$.^{24,25} This way of computing α_{xy} makes use of the Berry curvature in the graphene band structure [see Eq. (24)] more directly. It is a much more general method, which we have used in our plots for the Nernst coefficient as a function of temperature in Figs. 2 and 3. Using this method, we have been able to go beyond the linear temperature dependence arising out of the Mott relation.

The paper is organized as follows: Sec. II gives the Dirac-like Hamiltonian for single layer graphene. Section III is devoted to the topological Hall conductivity of single layer graphene. We calculate the ac Hall conductivity $\sigma_{ij}(\Omega)$ using the path-integral approach and discuss the possible polar Kerr effect for single layer graphene. In the limit $\Omega=0$, we obtain the dc Hall conductivity. The effects of nonlinear quasiparticle dispersion relation on the Hall conductivity are also discussed. In Sec. IV, we calculate the topological Nernst conductivity α_{xy} via both the Mott relation and the transverse heat current coefficient. We do this for both single and bilayer graphenes. Finally, Sec. V is devoted to the conclusion.

II. DIRAC-LIKE HAMILTONIAN

In the tight-binding approximation, graphene single layer with staggered sublattice potential (which breaks the space inversion symmetry) can be modeled with the nearest-neighbor hopping energy t and a site energy difference Δ between the sublattices,²⁶

$$H = \begin{pmatrix} \Delta/2 & \zeta(\mathbf{p}) \\ \zeta^*(\mathbf{p}) & -\Delta/2 \end{pmatrix}, \quad (1)$$

where

$$\zeta(\mathbf{p}) = -t \sum_i e^{i\mathbf{p} \cdot \delta_i} = -te^{ip_x a/2} \left[2 \cos\left(\frac{\sqrt{3}p_y a}{2}\right) + e^{-i3p_x a/2} \right] \quad (2)$$

with $\delta_{1,2} = \frac{a}{2}(1, \pm\sqrt{3})$, $\delta_3 = a(-1, 0)\hat{x}$, where a is the lattice constant. Hamiltonian (1) operates on the two-component

spinor $\hat{\Psi}_{\mathbf{p}} = (\hat{c}_{A\mathbf{p}}, \hat{c}_{B\mathbf{p}})$, where $\hat{c}_{A\mathbf{p}}, \hat{c}_{B\mathbf{p}}$ denote the annihilation operators on the two sublattices, A and B . The most interesting physics occurs around two valleys located at the Brillouin zone corners $\mathbf{K}_{1,2} = \frac{4\pi}{3\sqrt{3}a}(0, \tau_z)$, where $\tau_z = \pm 1$ labels the two valleys. Denoting $\mathbf{k} = \mathbf{p} - \mathbf{K}_{1,2}$ to measure the momentum from the valley centers, we can rewrite Hamiltonian (1) as

$$H = \frac{\Delta}{2} \sigma_z + \zeta_1(\mathbf{k}) \sigma_x + \zeta_2(\mathbf{k}) \sigma_y. \quad (3)$$

Here

$$\zeta_1(\mathbf{k}) = -t \left[2 \cos \frac{k_x a}{2} \cos \left(\frac{2\pi}{3} \tau_z + \frac{\sqrt{3}k_y a}{2} \right) + \cos(k_x a) \right], \quad (4)$$

$$\zeta_2(\mathbf{k}) = t \left[2 \sin \frac{k_x a}{2} \cos \left(\frac{2\pi}{3} \tau_z + \frac{\sqrt{3}k_y a}{2} \right) - \sin(k_x a) \right]. \quad (5)$$

The spectrum of the Hamiltonian consists of two branches with the eigenenergies $E_{\pm}(\mathbf{k}) = \pm \Lambda(\mathbf{k})$, where

$$\Lambda(\mathbf{k}) = \left[t^2 \left(1 + 4 \cos^2 \Theta + 4 \cos \Theta \cos \frac{3k_x a}{2} \right) + \frac{\Delta^2}{4} \right]^{1/2}, \quad (6)$$

$$\Theta = \frac{2\pi}{3} + \frac{k_y a \sqrt{3}}{2} \tau_z.$$

Close to the valley centers, we can expand $\zeta_1(\mathbf{k})$ and $\zeta_2(\mathbf{k})$ to the first order in \mathbf{k} and rewrite the Hamiltonian as

$$\hat{H} = \frac{\Delta}{2} \sigma_z + \frac{3at}{2} (\tau_z k_y \sigma_x - k_x \sigma_y) = \Lambda(\mathbf{k}) \cdot \sigma \quad (7)$$

with $\Lambda_1 = 3at\tau_z k_y/2$, $\Lambda_2 = -3atk_x/2$, and $\Lambda_3 = \Delta/2$. The energy spectrum becomes

$$\Lambda(\mathbf{k}) = |\Lambda(\mathbf{k})| = \frac{\sqrt{\Delta^2 + 9a^2 t^2 k^2}}{2}. \quad (8)$$

III. HALL CONDUCTIVITY

A. ac Hall conductivity

Introducing the Lagrangian density, $\mathcal{L} = i\omega_n \hat{I} - \hat{H}(\mathbf{k})$, where ω_n is a fermionic Matsubara frequency, we obtain the electron Green's function (for a single valley) as a function of $\vec{k} = (i\omega_n, k_x, k_y)$,

$$G_0(\vec{k}) = \mathcal{L}^{-1} = \frac{i\omega_n \hat{I} + \Lambda(\mathbf{k}) \cdot \hat{\sigma}}{g(\omega_n, \mathbf{k})}. \quad (9)$$

Here $g(\vec{k}) = (i\omega_n)^2 - |\Lambda(\mathbf{k})|^2$. In order to calculate the ac Hall conductivity, we consider the electromagnetic potential $\vec{A} = (A_0, A_x, A_y)$, where A_0 is the scalar potential and $\mathbf{A} = (A_x, A_y)$ is the vector potential. Expanding \mathcal{L} to the first order in \vec{A} and integrating out the fermions, we identify the coefficient of the Chern-Simons-like term in the effective action as the anomalous ac Hall conductivity for a single valley.²³

$$\sigma_{xy}(\Omega_m) = \sum_{\vec{k}} \frac{Y(\mathbf{k})}{g(\omega_n, \mathbf{k})g(\omega_n + \Omega_m, \mathbf{k})}, \quad (10)$$

$$Y(\mathbf{k}) = -2\Lambda \cdot \left[\frac{\partial \Lambda}{\partial k_x} \times \frac{\partial \Lambda}{\partial k_y} \right]. \quad (11)$$

Here the electromagnetic potential $\vec{A}(\vec{q})$ was assumed to be a function of the Fourier variables $\vec{q}=(i\Omega_m, q_x, q_y)$, with Ω_m as a bosonic Matsubara frequency, and we took the limit $\mathbf{q} \rightarrow 0$ to arrive at Eq. (10). Substituting the expression for $\Lambda(\mathbf{k})$ from Hamiltonian (7) into formula (11), we find

$$Y(\mathbf{k}) = \frac{-9\tau_z a^2 t^2 \Delta}{4}. \quad (12)$$

Summing over the fermionic Matsubara frequency ω_n in Eq. (10) and analytically continuing to the real bosonic frequency, $i\Omega_m \rightarrow \Omega + i\delta$, where δ is a positive infinitesimal, we find

$$\sigma_{xy}(\Omega) = \int \frac{d^2\mathbf{k}}{(2\pi)^2} \frac{Y(\mathbf{k})\{f[E_+(\mathbf{k}) - \mu] - f[E_-(\mathbf{k}) - \mu]\}}{\Lambda(\mathbf{k})[\Omega + i\delta - 2\Lambda(\mathbf{k})][\Omega + i\delta + 2\Lambda(\mathbf{k})]}. \quad (13)$$

Here $f(E - \mu)$ is the Fermi occupation function at temperature T and μ is the chemical potential. The minus sign between the two Fermi functions is due to the opposite sign of the Berry curvature for the conduction and the valence bands of electrons. Note that the ac Hall conductivity can also be calculated using Kubo formula,²⁷ which should yield the same results. Since $\Lambda(\mathbf{k}) = \sqrt{\Delta^2 + 9a^2 t^2 k^2}/2$ and $Y(\mathbf{k})$ are constants, we can define $\varepsilon = k^2/2$ and change the integration to

$$\sigma_{xy}(\Omega) = \int_0^\infty \frac{d\varepsilon}{2\pi E(\varepsilon)[\Omega + i\delta - 2E(\varepsilon)][\Omega + i\delta + 2E(\varepsilon)]}, \quad (14)$$

where $E(\varepsilon) = \frac{1}{2}\sqrt{\Delta^2 + 18a^2 t^2 \varepsilon}$, $F(\mu) = \{f[E(\varepsilon) - \mu] - f[-E(\varepsilon) - \mu]\}$.

It is clear that if the two valleys have the same chemical potential, $\mu_{K_1} = \mu_{K_2}$, the total ac Hall conductivity $\sigma_{xy}(\Omega) = \sigma_{xy}^{K_1}(\Omega) + \sigma_{xy}^{K_2}(\Omega) = 0$ because of the opposite signs of the function Y for the two valleys. However, the Hall current for an individual valley is nonzero.

The imaginary part of the ac Hall conductivity, $\sigma_{xy}''(\Omega)$, comes from the pole in Eq. (13) at $\Omega = 2E(\varepsilon)$. This pole represents vertical interband transitions induced by the electromagnetic wave. Taking the imaginary part of Eq. (13), we find

$$\sigma_{xy}''(\Omega) = -\frac{Y e^2}{\pi \Omega^2 \hbar} \int_0^\infty d\varepsilon \delta[\Omega - 2E(\varepsilon)] F(\mu). \quad (15)$$

Here we have already taken into account the spin degeneracy. At $T=0$, $F(\mu)=0$ if $E(\varepsilon) < \mu$ and $F(\mu)=1$ if $E(\varepsilon) > \mu$. Therefore, if $\Omega < 2\mu$ or $\Omega < \Delta$, $\sigma_{xy}''(\Omega)=0$. If $\Omega \geq 2\mu$ and $\Omega \geq \Delta$, we have

$$\sigma_{xy}''(\Omega) = \frac{e^2 \Delta}{2\hbar \Omega}. \quad (16)$$

At finite temperatures, we have $\sigma_{xy}''(\Omega) = \frac{\Delta e^2}{2\hbar \Omega} F(\mu)$ if $\Omega \geq \Delta$. For unequal population of the quasiparticles in the two valleys, the imaginary part of the ac Hall conductivity is nonzero. Since the polar Kerr angle, θ_K , which is the angle of rotation of the plane of polarization of a linearly polarized light on normal reflection from the sample, is directly proportional to $\sigma_{xy}''(\Omega)$,^{22,23} in this case, there will be a nonzero polar Kerr effect in graphene.

B. dc Hall conductivity

Taking $\Omega=0$ in Eq. (13), we have for the dc Hall conductivity

$$\sigma_{xy}(0) = - \int \frac{d^2\mathbf{k}}{(2\pi)^2} \frac{Y F(\mu)}{4\Lambda^3(\mathbf{k})}. \quad (17)$$

Notice that

$$\Pi = -\frac{Y}{4\Lambda^3(\mathbf{k})} = \frac{9a^2 t^2 \Delta \tau_z}{2(\Delta^2 + 9a^2 t^2 k^2)^{3/2}} \quad (18)$$

is just the Berry curvature for an individual valley.¹⁵ We see that the Berry curvatures for the two valleys differ only by a sign. At zero temperature and $\mu=0$, $\sigma_{xy}(0) = -\tau_z/4\pi$. We should multiply the result by two to take account of spin degeneracy. Restoring e and \hbar , we have (for a single valley)

$$\sigma_{xy}(0) = -e^2 \tau_z / h. \quad (19)$$

For nonzero $\mu > \Delta/2$, i.e., μ lying in the conductance band,

$$\sigma_{xy}(0) = -\tau_z e^2 \Delta / 2h\mu. \quad (20)$$

As μ becomes very big, $\sigma_{xy}(0)$ again becomes zero.

C. Nonlinear spectrum

The form of Berry curvature (18) $\Pi = -\frac{Y}{4\Lambda^3}$ also applies to general Hamiltonian (3) without the linear approximation [i.e., Hamiltonian (7)]. In this case, we should use Λ determined by Eq. (6). It is easy to show that

$$Y(\mathbf{k}) = -\frac{\sqrt{3}a^2 t^2 \Delta \tau_z}{2} \left[2 \cos\left(\frac{\pi}{6} + \frac{\sqrt{3}k_y a}{2} \tau_z\right) \cos\left(\frac{3k_x a}{2}\right) + \cos\left(\frac{\pi}{6} - \sqrt{3}k_y a \tau_z\right) \right]. \quad (21)$$

The lowest order in \mathbf{k} (i.e., $\mathbf{k}=0$) of Eq. (21) yields Eq. (12). In the presence of the nonlinear part of the spectrum, the symmetry relation between the Berry curvatures in the two valleys is given by $\Pi_{K_1}(\mathbf{k}) = -\Pi_{K_2}(-\mathbf{k})$, and the total Nernst conductivity will be nonzero only for nonzero valley polarization. In Fig. 1(a), we plot the Berry curvature around the valley center \mathbf{K}_2 ($\tau_z = -1$). We see that the Berry curvature is very small for a large \mathbf{k} . Therefore, the large \mathbf{k} regimes give very little contribution to the transport quantity of graphene. In fact, for $(k_x a, k_y a) = (\frac{\pi}{36}, \frac{\pi}{36})$, the Berry curvature is only

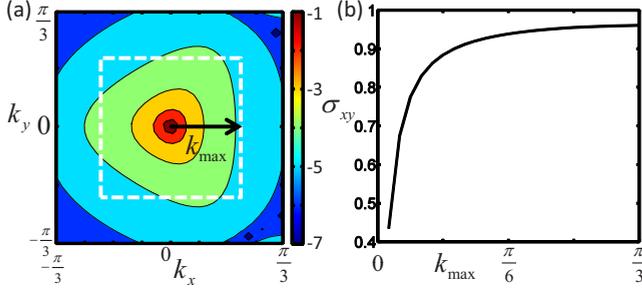


FIG. 1. (Color online) (a) Berry curvature Π (we plot $-\Pi$ for convenience) around the valley center K_2 . The parameters are $t = 2.8$ eV and $\Delta = 0.26$ eV. The plot is in the logarithm scale. The dashed line indicates the integration region for (b). (b) Plot of the dc conductivity with different integration regions, $-k_{\max} \leq k_x, k_y \leq k_{\max}$. The unit of $\sigma_{xy}(0)$ is e^2/h .

1% of its peak value. In Fig. 1(b), we plot the dc Hall conductivity at $T=0$ and $\mu=0$, taking account of the nonlinear spectrum. Because of the nonlinear spectrum, we cannot take the integration region up to $k=\infty$, the limit that is used for the linear spectrum. However, the dc Hall conductivity $\sigma_{xy}(0)$ at each valley is still very close to $-e^2\tau_z/h$ [the value in Eq. (19) obtained using the linear spectrum] for a reasonably large integration region. Therefore the nonlinear spectrum does not play an important role on the anomalous topological transport properties of graphene and will be neglected in the following.

IV. ANOMALOUS NERNST EFFECT

A. Single layer graphene

Since the transverse Hall conductivity can be nonzero for gapped graphene, it is natural to ask whether there exists an anomalous Nernst effect. For this purpose, at low temperatures, we can use the Mott relation,²¹

$$\alpha_{xy} = -\frac{\pi^2 k_B^2}{3e} \frac{d\sigma_{xy}}{d\mu} T. \quad (22)$$

For $-\Delta/2 < \mu < \Delta/2$, i.e., μ falling in the band gap, σ_{xy} is independent of μ , and we have $\frac{d\sigma_{xy}}{d\mu} = 0$. Thus, $\alpha_{xy} = 0$. If $\mu \geq \Delta/2$, we have

$$\frac{d\sigma_{xy}}{d\mu} = \frac{\tau_z e^2 \Delta}{2h\mu^2}. \quad (23)$$

Similarly, for $\mu \leq -\Delta/2$, $\frac{d\sigma_{xy}}{d\mu} = -\tau_z \frac{e^2}{h} \frac{\Delta}{2\mu^2}$. We see that α_{xy} is discontinuous at $\mu = \pm \Delta/2$.

More generally, the anomalous contribution to α_{xy} can be calculated from the transverse heat current coefficient $\bar{\alpha}_{xy}$. This way of computing α_{xy} makes direct use of the Berry curvature in the graphene band structure. In the presence of the Berry curvature and the electric field, the electron velocity acquires the additional anomalous term $\hbar \mathbf{v}_{\mathbf{k}} = e\mathbf{E} \times \Pi(\mathbf{k})$.²⁸ This velocity multiplied by the entropy density produces the transverse heat current coefficient,²⁹

$$\bar{\alpha}_{xy} = T\alpha_{xy} = \frac{2e}{\beta\hbar} \sum_n \int \frac{d^2\mathbf{k}}{(2\pi)^2} \Pi_n(\mathbf{k}) s_n(\mathbf{k}). \quad (24)$$

Here $s(\mathbf{k}) = -f_{\mathbf{k}} \ln f_{\mathbf{k}} - (1-f_{\mathbf{k}}) \ln(1-f_{\mathbf{k}})$ is the entropy density of the electron gas, $f_{\mathbf{k}} = f[E_n(\mathbf{k})]$ is the Fermi distribution function, and the sum is taken over both bands. This formula for α_{xy} , which we use in Figs. 2 and 3, coincides with the expression derived from Eq. (22) only at low temperatures. If $\mu_{K_1} = \mu_{K_2}$, we again see that $\alpha_{xy} = 0$ since the Berry curvature $\Pi_{K_1} = -\Pi_{K_2}$. However, the anomalous Nernst coefficient for each valley remains nonzero. The anomalous Nernst effect, for a uniform chemical potential, can therefore be used to create equal and opposite valley-index polarizations on the two transverse edges. This situation is similar to the analogous spin Hall effect³⁰ or possible valley Hall effect in graphene.¹⁵ For unequal chemical potential in the valleys,

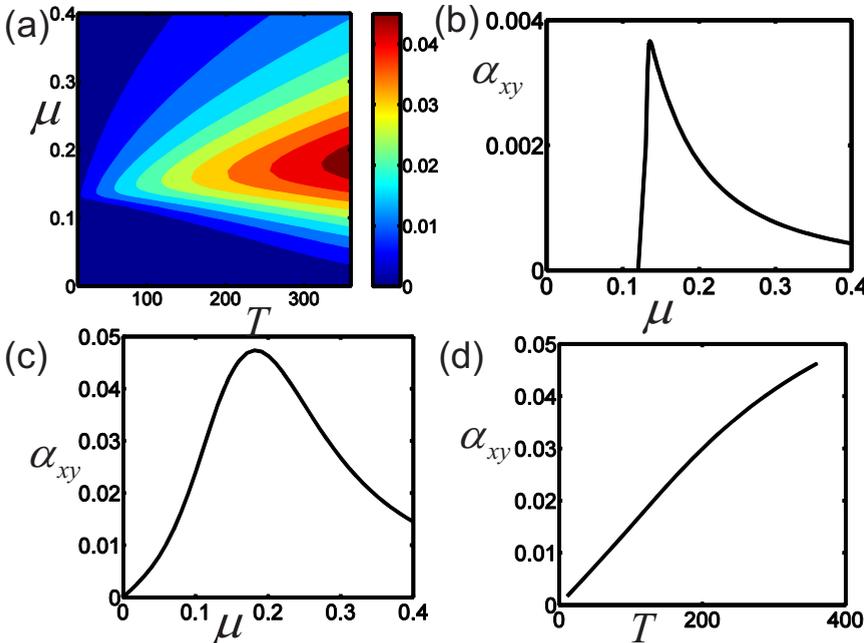


FIG. 2. (Color online) Anomalous Nernst signal for a single valley for single layer graphene. The units for μ , T , and α_{xy} are eV, K, and $k_B e/h$, respectively. The parameters are $t = 2.82$ eV and $\Delta = 0.26$ eV. (a) Contour plot for α_{xy} . (b) Plot of α_{xy} with respect to μ for $T = 11.6$ K. Note the discontinuity at $\mu = \Delta/2$ as predicted by the Mott relation. The decay for $\mu > \Delta/2$ follows $\sim 1/\mu^2$. (c) Plot of α_{xy} with respect to μ for $T = 360$ K. Note the disappearance of the discontinuity. (d) Plot of α_{xy} with respect to T for $\mu = 0.2$ eV.

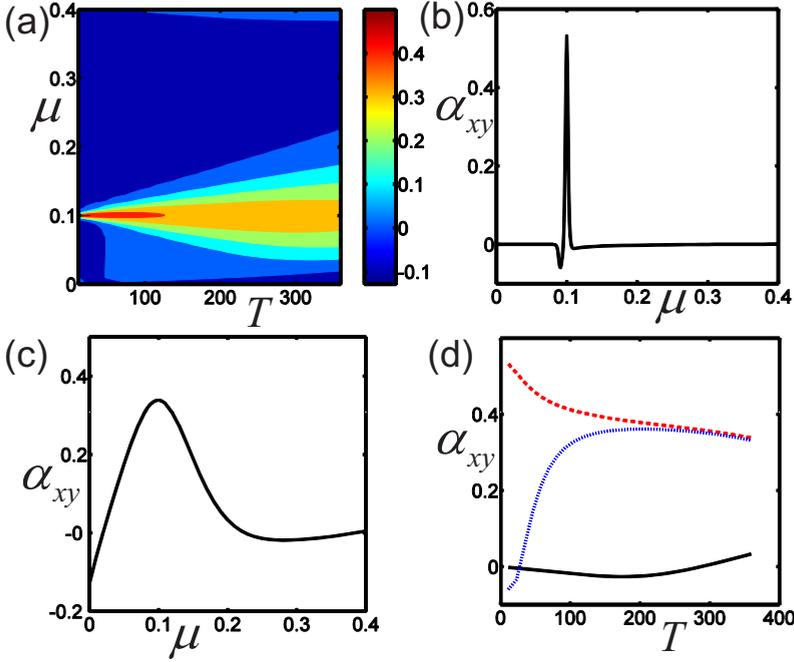


FIG. 3. (Color online) Anomalous Nernst signal for a single valley for bilayer graphene. The units for μ , T , and α_{xy} are eV, K, and $k_B e / \hbar$, respectively. The parameters are $t = 2.82$ eV, $V = 0.2$ eV, and $t_{\perp} = 0.4$ eV. (a) Contour plot for α_{xy} . (b) Plot of α_{xy} with respect to μ for $T = 11.6$ K. Note the dramatic variation in α_{xy} around $\mu = V/2$. (c) Plot of α_{xy} with respect to μ for $T = 360$ K. (d) Plot of α_{xy} with respect to T for $\mu = 0.2$ eV (solid line), 0.1 eV (dashed line), and 0.091 eV (dotted line).

which can be either artificially created¹⁹ or induced by a perpendicular magnetic field in a generic Nernst setup, there will be a nonzero anomalous contribution to the Nernst effect in graphene. The unequal valley chemical potential in the presence of an external magnetic field is due to the Zeeman-type coupling of the magnetic field with the substantial magnetic moment associated with the valleys, which can be 30 times bigger than the usual spin magnetic moment.¹⁵

Since Eq. (24) is more general than the Mott relation and may be used to go beyond the linear temperature dependence of α_{xy} [Eq. (22)], we numerically evaluate Eq. (24) to calculate the Nernst coefficient. We plot the anomalous Nernst coefficient as a function of μ and T for a single valley in single layer graphene in Fig. 2. In Fig. 2(a), there is a nonzero Nernst coefficient even when the chemical potential is inside the band gap, while the Mott relation yields a zero Nernst signal in this case. In Fig. 2(b), Nernst conductivity α_{xy} increases sharply to a maximum, while the Mott relation yields a step jump at $\mu = \frac{\Delta}{2}$. In Fig. 2(c), the step jump is further smoothed out at medium temperatures (note that T here is still much smaller than Δ). The deviation of α_{xy} from the linear temperature dependence given by the Mott relation is clearly visible in Fig. 2(d).

B. Anomalous Nernst effect in bilayer graphene

The Hamiltonian for a single valley in biased bilayer graphene can be written as²⁶

$$\hat{H} = \begin{pmatrix} V/2 & tke^{i\phi_{\mathbf{k}}} & t_{\perp} & 0 \\ tke^{-i\phi_{\mathbf{k}}} & V/2 & 0 & 0 \\ t_{\perp} & 0 & -V/2 & tke^{-i\phi_{\mathbf{k}}} \\ 0 & 0 & tke^{i\phi_{\mathbf{k}}} & -V/2 \end{pmatrix}, \quad (25)$$

where V is the interlayer bias voltage, t_{\perp} and t describe interlayer and intralayer nearest-neighbor hoppings, and $\phi_{\mathbf{k}}$ is

the angle of \mathbf{k} on the two-dimensional momentum space. The eigenenergies and eigenstates can be obtained analytically, which yield the Berry curvature for the n th band,

$$\Pi_n = \frac{1}{k} \frac{\partial}{\partial k} [A_n^2 (\gamma_{1n}^2 - \gamma_{3n}^2)]. \quad (26)$$

Here $A_n = (1 + \gamma_{1n}^2 + \gamma_{2n}^2 + \gamma_{3n}^2)^{-1/2}$, $\gamma_{1n} = tk / (E_n - V/2)$, $\gamma_{2n} = -[t^2 k^2 / (E_n - V/2) - (E_n - V/2)] / t_{\perp}$, $\gamma_{3n} = \gamma_2 tk / (E_n + V/2)$, and finally

$$E_n = \pm \frac{1}{2} \sqrt{2t_{\perp}^2 + V^2 + 4t^2 k^2 \pm 2\sqrt{4(V^2 + t_{\perp}^2)t^2 k^2 + t_{\perp}^4}} \quad (27)$$

are the eigenenergies.

In Fig. 3, we plot α_{xy} as a function of μ and T , similar as in Fig. 2. Note that, in this case, α_{xy} can change sign in some regimes of the parameter space. Such sign changes are due to the complicity of the four bands of bilayer graphene. At low temperatures, $\alpha_{xy} = 0$ for $\mu < V/2$ and changes dramatically around $\mu = V/2$. The dramatic change in α_{xy} disappears at medium temperatures, but the sign change still remains [see Fig. 3(c)]. At different chemical potentials, the temperature dependence of α_{xy} shows quite different behaviors [see Fig. 3(d)]. For uniform chemical potential at the valleys, the total anomalous Nernst signal is zero even though, like in the case of single layer graphene, they can be substantial locally in the momentum space.

V. CONCLUSION

In summary, we discuss the effects of the topological Berry phases on the thermoelectric response coefficients of the Dirac-like quasiparticles in gapped single and bilayer graphene. The gap in the single layer graphene can be due to SI symmetry breaking, as claimed, for instance, in epitaxial

graphene in Ref. 9. It may also be due to confined geometries, such as in graphene nanoribbons.^{10,11} For bilayer graphene, the gap may be due to applied voltage bias.¹² We show that in such samples the anomalous contribution to the Nernst effect is nonzero for a nonzero valley polarization. We also show that the nonlinear quasiparticle dispersion spectrum does not significantly change the results. A nonzero valley polarization may be artificially created,¹⁹ or it can be induced by a perpendicular magnetic field due to the substantial valley magnetic moment¹⁵ in a generic Nernst setup. The regular Nernst effect in gapped graphene may, therefore, have a substantial anomalous contribution because of the

valley polarization. Even in the absence of any valley polarization, the spontaneous Nernst effect from an individual valley is locally nonzero, opening up the possibility to create a measurable valley polarization on the transverse edges of a sample which can be technologically very important.

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