Anomalous thermo-spin effect in the low-buckled Dirac materials

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A strong spin Nernst effect with nontrivial dependences on the carrier concentration and electric field applied is expected in silicene and other low-buckled Dirac materials. These Dirac materials can be considered as made of two independent electron subsystems of the two-component gapped Dirac fermions. For each subsystem the gap breaks a time-reversal symmetry and thus plays a role of an effective magnetic field. Accordingly, the standard Kubo formalism has to be altered by including the effective magnetization in order to satisfy the third law of thermodynamics. We explicitly demonstrate this by calculating the magnetization and showing how the correct thermoelectric coefficient emerges.

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Introduction. —The thermoelectric and thermomagnetic phenomena discovered in the nineteen century turned out unexpectedly to be in the spotlight at the beginning of the twenty first one. First of all, from the practical point of view, control of the heat fluxes and minimization of the related losses are important factors for designing modern elements of nanoelectronics. At the same time, the discovery of Nernst-Ettinghausen (NE) signal hundred times larger than its normal value in the pseudogap phase of high temperature superconductor La$_2$-xSr$_x$CuO$_4$, followed by a similar finding (with $10^3$ enhancement in magnitude) in the fluctuating regime of conventional superconductor Nb$_{0.15}$Si$_{0.85}$, indicated on a sensible and powerful tools for study of microscopic properties of novel systems. In graphene where the Dirac point can be crossed by tuning the position of the chemical potential, a huge compared to the nonmagnetic materials SN effect even in the ab-normal conductor subjected to a magnetic field. It is the quantum spin Hall (QSH) effect becomes experimentally accessible in graphene. The later is fundamentally related to the anomalous Hall effect in ferromagnets. The analogy between thermomagnetic phenomena in graphene and spintronics of the low-buckled Dirac materials shows that the last ones should also be very promising for the investigation of the spin caloritronics phenomena.

Due to nonzero spin-orbit gap $\Delta_{SO}$ the quantum spin Hall (QSH) effect becomes experimentally accessible in silicene. The analogy between thermomagnetic phenomena in graphene and spintronics of the low-buckled Dirac materials shows that the last ones should also be very promising for the investigation of the spin caloritronics phenomena. Among them special interest represents the off-diagonal spin Nernst (SN) effect, an analogue of the NE effect in ferromagnets. The analogy between thermomagnetic phenomena in graphene and spintronics of the low-buckled Dirac materials shows that the last ones should also be very promising for the investigation of the spin caloritronics phenomena.

In this context the synthesis of silicene, a monolayer of silicon atoms forming a two-dimensional low-buckled lattice, boosted theoretical studies of a wide class of new Dirac materials. The honeycomb lattice of silicene can be described as in graphene in terms of two triangular sublattices. However, a larger ionic size of silicon atoms results in buckling of the 2D lattice. Accordingly, the sites on the two sublattices are vertically separated on the distance $2d \approx 0.46\AA$. Consequently, silicene is expected to have a strong intrinsic spin-orbit interaction that results in a sizable spin-orbit gap, $\Delta_{SO}$, in the quasiparticle spectrum opened at the Dirac points. Moreover, by applying the perpendicular to the plane electric field $E_z$ it is possible to create the on-site potential difference between the two sublattices opening the additional gap, $\Delta_z = E_z d$ in the quasiparticle spectrum. Similar structure and properties are also expected in 2D sheets of Ge, Sn, P and Pb atoms (the first three materials are coined as germanene, stanene and phosphorene).

In this letter we will show that due to the large value of $\Delta_{SO} \sim 10\text{meV}$, the off-diagonal thermo-spin coefficient, $\beta_{xy}$, is indeed expected to be huge in these materials simultaneously being nontrivially dependent on the chemical potential $\mu$ and electric field $E_z$.

Silicene model. —The low-energy physics of silicene is described by the Hamiltonian density

$$
\mathcal{H}_\xi = \sigma_0 \otimes \left[ \hbar v_F (\xi k_x \tau_1 + k_y \tau_2) + \Delta_z \tau_3 - \mu \tau_0 \right] - \xi \Delta_{SO} \sigma_3 \otimes \tau_3,
$$

where the Pauli matrices $\tau, \sigma$, and the unit matrices, $\tau_0$ and $\sigma_0$ act in the sublattice and spin spaces, respectively, and the wavevector $k$ is measured from the $K_\xi$ points.
with \( \xi = \pm \). Here we neglected the small Rashba interaction [27]. The Hamiltonian [1], describes four kinds (two identical pairs) of the noninteracting massive (gapped) Dirac quasiparticles with the masses \( \Delta \xi_{\sigma}/v_{F} \), where \( v_{F} \) is the Fermi velocity, \( \sigma(= \pm) \) is the spin, and valley \( \xi \) dependent gap \( \Delta \xi_{\sigma} = \Delta_{z} - \xi \sigma \Delta_{SO} \).

The QSH effect in silicene occurs due to the presence of two subsystems with \( \sigma = \pm \) exhibiting the quantum Hall effect. The corresponding chiral edge states are spin polarized and form a time-reversed pair to recover the overall time-reversal symmetry (the Kane-Mele scenario [29]). The spin Hall conductivity can be expressed in terms of the electric Hall conductivity \( \sigma_{xy}(\Delta) \) for the two-component Dirac fermions with the gap \( \Delta \) (see the Hamiltonian [30] below) by the relation

\[
\sigma_{xy} = \frac{-\hbar}{2e} \sum_{\xi, \sigma = \pm} \xi \sigma \sigma_{xy}(\Delta \to \Delta \xi_{\sigma}).
\]

The factor \(-\hbar/2e\) indicates that in the off-diagonal correlation function of the two electric currents one electric current is replaced by the spin current.

Being subjected to the temperature gradient \( \nabla T \) the spin polarized chiral edge states lose their time-reversal symmetry and the spin current \( j^{s} \) flows. The latter is related to \( \nabla T \) by means of the thermo-sensor, \( \beta^{s} \), via \( \beta^{s} j^{s} = -\beta \nabla T \). Analogously to the spin Hall conductivity, the off-diagonal component \( \beta_{xy}^{s} \) can be obtained from (2) by substitution \( \sigma_{xy}^{s} \to \beta_{xy}^{s} \) and \( \sigma_{xy}(\Delta) \to \beta_{xy}(\Delta) \), where \( \beta_{xy}(\Delta) \) is the standard thermoelectric coefficient for the two-component Dirac fermions. Thus in the absence of valley mixing the study of the spin transport coefficient is reduced to the investigation of the electric transport for the two-component gapped Dirac fermions. – The corresponding Hamiltonian density is

\[
\mathcal{H} = \hbar v_{F}(k_{x} \tau_{1} + k_{y} \tau_{2}) + \Delta \tau_{3} - \mu \tau_{0}.
\]

This model with broken time-reversal symmetry provides a simple realization of the anomalous Hall and thermoelectric effects. Its main merit is the possibility of obtaining simple approximate analytical expressions in the presence of spin-independent random potential with Gaussian correlations [23, 28, 30].

Qualitative analysis. — A qualitative evaluation of the thermoelectric coefficient \( \beta_{xy}(\Delta) \) can be obtained basing on the Mott relation,

\[
\beta_{xy} = \frac{\pi^{2}k_{B}^{2}}{3e} \frac{T}{T} \frac{\partial \sigma_{xy}(\mu, \Delta, T = 0)}{\partial \mu},
\]

where \( k_{B} \) is the Boltzmann constant. In the clean limit at \( T = 0 \) one finds [28, 30]

\[
\sigma_{xy} = -\frac{e^{2} \text{sgn} \Delta}{4\pi \hbar} \begin{cases} 1, & |\mu| \leq |\Delta|, \\
|\Delta|/|\mu|, & |\mu| > |\Delta|,
\end{cases}
\]

wherefrom we can make two conclusions.

i) For \(|\mu| > |\Delta| \) we obtain that \( \beta_{xy} = -(k_{B}/e)(\pi \epsilon^{2}/12\hbar)(\Delta \text{sgn} \mu/\mu^{2})k_{B}T \). Then the Nernst signal \( e_{y}(T) \equiv -E_{y}/\nabla_{x} T \), where \( E_{y} \) is the electric field in \( y \)-direction, can be estimated as

\[
e_{y}(T) \approx \frac{\beta_{xy}}{\sigma_{xx}} = -\frac{k_{B}}{e} \frac{\pi \epsilon^{2}}{12\hbar \sigma_{xx} \mu^{2}} \Delta k_{B} T \text{sgn} \mu.
\]

Here we assumed that the diagonal conductivity, \( \sigma_{xx} \gg |\sigma_{xy}| \).

The main feature of the Dirac materials is that the value of the chemical potential \( \mu \) can be tuned as close as possible to the regime with \( e_{y}(T) \sim k_{B}/e \sim 86 \mu V/K \). This is exactly how one gains from 3 to 4 orders of magnitude in the Nernst signal as compared to the normal nonmagnetic metals, where \( e_{y} \) is negligibly small (~10 nV/K per Tesla).

ii) Our simple estimate also shows that the Mott’s formula fails near \(|\mu| = |\Delta| \) when the conductivity \( \sigma_{xy}(\mu, \Delta, T) \) changes abruptly. Indeed, as discussed recently in [8] (see also references therein) when the gap is present in the quasiparticle spectrum, one should use the microscopic approach. The same concerns the SN effect: to the best of our knowledge so far it was studied exclusively using the analog of the Mott’s formula written for the spin conductivity [31].

Modified Kubo formula. — The study of the off-diagonal thermal transport in the framework of the Kubo formalism is a delicate issue. It was firstly understood fifty years ago by Obraztsov [32] that side by side with the Kubo-like response on the temperature gradient the magnetization currents must be taken into account in order to satisfy the Onsager principle of the symmetry of the kinetic coefficients. It worthwhile to mention that this problem has been readdressed practically each decade [33–37] due to its importance for the quantum Hall effect, NE in fluctuating superconductors, etc. In the problem under consideration the account for magnetization currents turns out to be crucial not only in order to get the correct coefficient in \( \beta_{xy} \) for the two-component gapped Dirac fermions, but first of all for the validity of the third law of thermodynamics.

In a view of the mentioned above, the Kubo formula for the off-diagonal thermal transport coefficient \( \beta_{xy} = -(\hbar/T) \lim_{\omega \to 0} Q_{xy}^{eq}(\omega) / \omega \) (here \( Q_{xy}^{eq}(\omega) \) is the retarded response function of electric and heat currents) in the presence of effective magnetic field has to be enriched with the corresponding magnetization \( M_{z} \), so that \( \beta_{xy} = \beta_{xy} + c M_{z}/T \).

The introduced above electric-heat currents linear response function in the Matsubara representation can be
presented as the bubble of two Green’s functions (GF)

\[
Q^{eq}_{\alpha\beta}(\Omega_m) = \sum_{\epsilon_n} \int \frac{d^2k}{(2\pi)^2} \text{tr} \left[ \Gamma^{(e)}_{\alpha}(\epsilon_n + \Omega_m, \epsilon_n) \right] \times G(\epsilon_n + \Omega_m, k) \gamma^{(q)}_{\beta}(\epsilon_n, \epsilon_n + \Omega_m) G(\epsilon_n, k)
\]

(7)

Here \( G(\epsilon_n, k) \) is the unboundedness of the electromagnetic energy, \( i(\epsilon_n + \Omega_m/2) \) is the time-reversal symmetry, the intrinsic magnetization is indeed expected to be nonzero. However, an attempt to derive a coordinate operator \( \hat{M} \) and references therein). It is the unboundedness of the magnetic field in the model (3) that does not allow \( M_z \) to be directly calculated. Having the GF it is already straightforward to calculate the carrier density \( \rho(\mu, T, B) \). The thermodynamic potential \( \Omega(\mu, T, B) \) can be obtained by integrating the relationship \( \rho = -\partial \Omega/\partial \mu \) over \( \mu \). Finally the magnetization \( M_z = -\partial \Omega/\partial B \). When \( T \gg \Gamma_0 \) it takes especially simple form

\[
\frac{M_z}{T} = \frac{e \text{sgn} \Delta}{4\pi \hbar c} \left[ \ln \cosh \frac{\mu + |\Delta|}{2k_BT} - \ln \cosh \frac{\mu - |\Delta|}{2k_BT} \right].
\]

(10)

Remarkably that in the limit \( T \rightarrow 0 \) the asymptotic of Eq. (10) up to a sign coincides with Eq. (5). This restores the validity of the third law of thermodynamics. Since \( \beta_{xy} \) describes the transversal entropy transport it must identically turn zero at \( T = 0 \). Eq. (10) illustrates in a spectacular way how the gap induces the anomalous magnetic moment.

Finally the off-diagonal transport coefficients \( \sigma_{xy}(\Delta) \) and \( \beta_{xy}(\Delta) \) can be presented in the standard form

\[
\begin{align*}
\sigma_{xy}(\Delta) &= \frac{e^2}{h} \int \frac{d\epsilon}{-\infty} \left[ -\frac{\partial f(\epsilon)}{\partial \epsilon} \right] \left\{ \frac{-1}{\epsilon} \right\} A_H(\mu + \epsilon, \Delta),
\end{align*}
\]

(11)

where all specific information about the model and the character of elastic scattering is contained in the zero temperature Hall conductivity \( \sigma_{xy}(\mu, \Delta, T = 0) = -e^2/h \). The analogous result was obtained by Smrčka and Štreda [32] for nonrelativistic fermions in magnetic field.

Two-component Dirac fermions: the results. — In the clean case, in the bubble approximation the function \( A_H(\mu, \epsilon, \Delta) \) with the level broadening acquires the form

\[
A^{(d)}_{H}(\epsilon, \Delta) = \frac{\Delta}{4\pi^2} \left[ \frac{1}{\epsilon} \left( \frac{\arctan |\Delta| + \epsilon}{\Gamma_0} - \arctan |\Delta| - \epsilon \right) \right] + \frac{1}{|\Delta|} \left( \frac{\arctan \frac{\epsilon + |\Delta|}{\Gamma_0} - \arctan \frac{\epsilon - |\Delta|}{\Gamma_0}}{\tan \frac{|\Delta|}{\Gamma_0}} \right).
\]

(12)

Accordingly, for \( T \rightarrow 0 \) (but \( T \gg \Gamma_0 \)) we obtain

\[
\beta^{(d)}_{xy}(\Delta) = -\beta_0 \frac{\pi k_B T}{12} \frac{\text{sgn} \mu}{\mu^2} \theta(\mu^2 - \Delta^2),
\]

(13)

where \( \beta_0 = k_B e/\hbar \). It is easy to see that Eq. (13) also directly follows from the Mott relation (4) and the conductivity (5). However, the general expression (11) allows us to investigate the vicinity of the point \( |\mu| = |\Delta| \), where the Mott result (13) fails.

The influence of disorder on Hall conductivity of the gapped Dirac fermions was studied in [28, 30]. The authors found the dressed vertex \( \gamma^{(v)}_{\beta}(\epsilon) \) in the ladder approximation. Accordingly, in the presence of disorder the kernel \( A_H(\mu, \epsilon, \Delta) \) takes the form

\[
\begin{align*}
A^{(d)}_{H}(\epsilon, \Delta) &= \frac{\text{sgn} \Delta}{4\pi} \theta(\Delta^2 - \epsilon^2) + \frac{\Delta}{4\pi |\epsilon|} \\
&\times \left[ 1 + \frac{4(\Delta^2 - \epsilon^2)}{\epsilon^2 + 3\Delta^2} + \frac{3(\epsilon^2 - \Delta^2)^2}{(\epsilon^2 + 3\Delta^2)^2} \right] \theta(\epsilon^2 - \Delta^2).
\end{align*}
\]

(14)
The important feature of \( A_{H}^{(cl)} \) is that in contrast to \( A_{H}^{(d)} \) it is independent of the disorder potential strength and of the concentration of impurities encoded in the scattering rates \( \Gamma_{0}(\epsilon) \) and \( \Gamma_{1}(\epsilon) \). Comparing the kernels \( A_{H}^{(d)} \) and \( A_{H}^{(cl)} \) one can see that the approximation of the disorder effects by the level broadening is insufficient even in the weak disorder limit [28, 30] and leads to the drastic changes in the behavior of \( \sigma_{xy} \) and \( \beta_{xy} \).

The dependencies \( \sigma_{xy}(\mu) \) and \( \beta_{xy}(\mu) \) are plotted in the left and right panels of Fig. 1 respectively. The dashed (red) and the solid (blue) curves correspond to the calculations done using the kernels \( A_{H}^{(cl)} \) and \( A_{H}^{(d)} \), respectively. We took \( T = 0.1\Delta \) and \( \Gamma_{0} = 0.05\Delta \). One can see that \( \sigma_{xy} \) and \( \beta_{xy} \) are even and odd functions of \( \mu \), respectively. On the opposite, in the case of a real magnetic field \( \sigma_{xy} \) and \( \beta_{xy} \) are odd and even functions of \( \mu \), respectively. In this respect a positive sign of the Nernst signal near \( \mu = 0 \) is regarded as one of the fingerprints of the Dirac quasiparticles. [3] In the case of the anomalous Hall and Nernst effects the sign of \( \beta_{xy} \) also remains very informative. One can see that the presence of the disorder vertex drastically changes the pattern of the sign changes in \( \beta_{xy}(\mu) \). The nonmonotonic dependence of \( \sigma_{xy}(\mu) \) on the electron \( \mu > 0 \) or hole \( \mu < 0 \) parts of carriers results in new nontrivial zeros of \( \beta_{xy}(\mu) \). Using the Mott relation one finds that these zeros are at \( \mu = \pm \sqrt{3 + 2\sqrt{3} |\Delta|} \approx \pm 2.5 |\Delta| \).

The results for silicene. — We return now to the discussion of the full model [1]. We calculate the spin Hall conductivity \( \sigma_{xy}^{S} \) from Eq. (2) and the thermo-spin coefficient \( \beta_{xy}^{S} \) from its analog using Eq. (11) for the two-component Dirac fermions.

For a reference, we begin with the kernel \( A_{H}^{(cl)} \). The spin Hall conductivity at \( T = 0 \) and zero sublattice asymmetry gap \( \Delta = 0 \) directly follows from Eq. (1) and reads

\[
\sigma_{xy}^{S} = -\left( e^{2}/4\pi \right) \text{sgn} \Delta_{SO} \theta(\Delta_{SO} - |\mu| + |\Delta_{SO}|/|\mu|) \theta(|\mu| - |\Delta_{SO}|).
\]

Then for the same case the thermo-spin coefficient \( \beta_{xy}^{S} \) is given by Eq. (13) with \( \Delta \) replaced by \( \Delta_{SO} \) and \( \beta_{0}' = k_{B}/2 \). Obviously, all stated above concerning a large Nernst signal for the model [5] turns out to be applicable for the SN effect in silicene.

We present the dependences \( \sigma_{xy}^{S}(\mu) \) and \( \beta_{xy}^{S}(\mu) \) computed using the kernel [11] for a general case \( \Delta_{z} \neq 0 \) in the left and right panels of Fig. 2. The case with the

FIG. 1: (Color online) Left panel (a): electrical Hall conductivity \( \sigma_{xy}(\mu) \) in units of \( \sigma_{0} = e^{2}/(4\pi h) \); right panel (b): thermoelectric coefficient \( \beta_{xy}(\mu) \) in units of \( \beta_{0}' = k_{B}/2 \) as functions of the chemical potential \( \mu \) in the units of \( \Delta > 0 \).

FIG. 2: (Color online) Left panel (a): spin Hall conductivity \( \sigma_{xy}^{S}(\mu) \) in units of \( \sigma_{0} = e^{2}/(2\pi h) \); right panel (b): thermo-spin coefficient \( \beta_{xy}^{S}(\mu) \) in units of \( \beta_{0}' = k_{B}/2 \) as functions of the chemical potential \( \mu \) in the units of \( \Delta_{SO} > 0 \).
FIG. 3: (Color online) Top panel: (a): spin Hall conductivity $\sigma_{xy}^{s}$ in units of $\sigma_{0}^{s}$; bottom panel (b): thermo-spin coefficient $\beta_{xy}^{s}$ in units of $\beta_{0}^{s}$ as functions of the chemical potential $\mu$ and the sublattice asymmetry gap $\Delta_{z}$ in the units of $\Delta_{SO} > 0$.

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