Thermoelectric relations in the conformal limit in Dirac and Weyl semimetals

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In the Fermi liquid (FL) description of metals, electrical and thermoelectric transport coefficients are linked by robust relations which can be challenged by strong interactions or when the electron liquid enters a different regime. These relations have been very powerful in the characterisation of novel materials. We show that Dirac and Weyl semimetals at zero doping and zero temperature (the conformal limit) have a very singular behavior due to a quantum anomaly. Away from this point, a Mott relation can be established.

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Leaving aside the important technological applications, thermal and electrothermal transport are very useful tools to characterise the physical properties of new materials [1]. In standard metals where almost free quasiparticles transport both electric charge and entropy, there are tight phenomenological relations between the various transport coefficients. Violations of these are used as signals of non-Fermi liquid behavior or to the appearance of new phases of the system.

An external electric field $\mathbf{E} = \nabla V$ or a temperature gradient $\nabla T$ induce electric and heat currents that in linear response can be written as:

$$
\begin{pmatrix}
J_i \\
J'_i
\end{pmatrix} = \begin{bmatrix}
\sigma_{ij} & \alpha_{ij} \\
T \tilde{\alpha}_{ij} & \kappa_{ij}
\end{bmatrix} \begin{pmatrix}
E_i \\
-\nabla_j T
\end{pmatrix},
$$

(1)

where $\sigma$, and $\kappa$ are the electric and thermal conductivity tensors respectively, and $\alpha$ is the thermoelectric coefficient. In the presence of a magnetic field (in the chosen direction OZ), the various tensors in eq. (1) can have time-reversal odd off-diagonal components as the Hall conductivity $\sigma_{xy}$ or the transverse thermopower $\alpha_{xy}$.

The best known phenomenological laws used in thermo-electrical transport are the Wiedemann-Franz (WF) law and the Mott relation [2]:

$$
\sigma_{ij} = T L \kappa_{ij}, \quad \alpha_{ij} = T L e \left( \frac{d\sigma_{ij}}{d\mu} \right)_{\mu = \epsilon_F}.
$$

(2)

The first one establishes that the ratio of the thermal to the electrical conductivity is the temperature times a universal number, the Lorenz number $L = \pi^2 k_B^2 / 3e^2$, where $k_B$ and $e$ are the Boltzmann constant and the unit charge. The Mott relation relates the thermopower tensor $\alpha$ with the temperature times the value of the derivative of the electrical conductivity with respect to the chemical potential at the Fermi level. The validity of these laws has been derived for any system which can be described as a Fermi liquid, provided the quasiparticles do not exchange energy during collisions. It has also been proven to be valid when a semiclassical description of the electronic system is allowed. Deviations from these phenomenological relations in conventional matter are normally attributed to electron–electron interactions inducing departures from Fermi liquid behavior or to the emergence of a new phase regime [3–5].

Typically Dirac materials in two and three dimensions are expected to follow the standard relations in the low T regime and deviate from it at larger temperatures [6–8]. Alternative descriptions of the novel Dirac materials reveal the presence of a hydrodynamic regime where departures from the standard FL behavior are also found [5, 9].

An interesting question arose associated to topological materials. These have anomalous conductivities (particularly Hall conductivity) similar to that occurring in ferromagnetic materials induced by the Berry curvature of the bands. The validity of the Mott relation for the anomalous transport phenomena was observed in films of Ga$_{1-x}$Mn$_x$As, a ferromagnetic semiconductor in [10]. The question of whether or not these anomalous transport coefficients obeyed the WF and Mott relations, arose soon after the recognition of topological properties. Berry curvature effects were cleverly added in the Boltzmann transport formalism in a way to fulfil the rules of Ga$_{1-x}$Mn$_x$As, a ferromagnetic semiconductor in [10]. The thermoelectric properties of Dirac and Weyl semimetals are a very active field of actual research [6, 16–18]. The influence of lattice deformation on the thermoelectric transport properties in Weyl semimetals has been discussed in [19].

In a recent work [20], a contribution to the Nernst current of a Dirac or Weyl semimetal coming from the conformal anomaly was reported. Being originated from an anomaly - a vacuum contribution -, a non-zero transport coefficient was predicted at zero temperature and chemical potential where the theory is scale invariant at the classical level. A Kubo formula calculation of the thermoelectric coefficient extended the calculation to finite temperature and chemical potential and gave the same result in the conformal limit [21]. In what follows we...
analyze the Mott relation in the light of the results in [20, 21]. The expression obtained in these references for the thermopower coefficient in eq. (1), for a single Dirac cone in three dimensions (in the geometry $B_z$, $\nabla_T$) was

$$\alpha^{xy} = \frac{e^2v_FB}{4\pi^2\hbar T}. \quad (3)$$

As highlighted in the original references, the coefficient $\alpha$ has a finite contribution from the conformal anomaly in the conformal limit (zero temperature and chemical potential). This is the most unusual behavior which automatically implies violation of the Mott relation in eq. (2). As we will see below, away from this singular point, the system has a standard - Fermi liquid-like - behavior.

In order to analyze the validity of the thermoelectric relations in the conformal limit of Dirac and Weyl matter, we calculate the Hall conductivity with a Kubo formulation as the one done in [21] for the thermopower. The calculation is straightforward but lengthy. The result for the Hall conductivity for a Weyl semimetal (in the local and zero frequency limit) is given by the expression:

$$\sigma^{xy} = \lim_{\eta \to 0} \sum_{N=M-1} \frac{1}{4\sqrt{2\pi}} \frac{e^2}{\hbar B} \int d\kappa_z \frac{-2\alpha_{k_z ms}^2}{(\alpha_{k_z ms}^2 + 1)(\alpha_{k_z ns}^2 + 1)} \left[ n_{k_z ms} - n_{k_z ns} \right]^2,$$

where the factor $[\alpha_{k_z ms}^2 + 1]^{1/2}$ comes from the wavefunction normalization of the Landau eigenvectors and is given by

$$\alpha_{k_z ms} = \frac{-\sqrt{2eBhM}}{E_{k_z ms}/sv_F - \hbar k_z} \quad (7)$$

and we have introduced the dimensionless variables $\sqrt{2eBh} = \hbar k_z$, $\epsilon_{k_z ms} = E_{k_z ms}/\hbar \omega_c$ ($\omega_c$ is the cyclotron frequency).

Figure 1 (a) shows the Landau level (LL) structure of a single chirality in a Dirac or Weyl semimetal. The blue straight line represents the chiral zeroth LL. The inset shows the thermoelectric coefficient computed in ref. [21]. It is related with that in (1) by $\chi^{xy} = \alpha^{xy}/T$. Right hand side: Hall conductivity $\sigma^{xy}$ as a function of the chemical potential in the range $-\hbar \omega_c \leq \mu \leq \hbar \omega_c$ for various values of the temperature.

FIG. 1: Left hand side: Landau level structure of a single chirality in a Dirac semi-metal. The blue straight line represents the chiral zeroth LL. The inset shows the thermoelectric coefficient computed in ref. [21]. It is related with that in (1) by $\chi^{xy} = \alpha^{xy}/T$. Right hand side: Hall conductivity $\sigma^{xy}$ as a function of the chemical potential in the range $-\hbar \omega_c \leq \mu \leq \hbar \omega_c$ for various values of the temperature.

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Figure 1 (a) shows the Landau level (LL) structure of a single chirality in a Dirac or Weyl semimetal. The blue straight line represents the chiral zeroth order LL. The inset shows the zero temperature thermoelectric coefficient $\chi = \alpha/T$ as a function of the chemical potential computed in ref. [21]. The function has a constant value when $\mu$ lies in the interval between the first Landau levels $n = \pm 1$. Figure 1(b) shows the the Hall conductivity $\sigma^{xy}$ as a function of the chemical potential for the same interval $-\hbar \omega_c \leq \mu \leq \hbar \omega_c$ and for various values of the temperature. The conductivity is linear at $T = 0$ where the main contribution comes from the lowest Landau level. As the temperature increases, the slope decreases and the function becomes smoother due to the contribution of the thermally activated carriers at higher Landau levels.

The derivative of the conductivity $\partial_\mu \sigma^{xy}$ at the Fermi surface $\mu = 0$ as a function of the temperature is depicted in Figure 2(a). The thermoelectric response function $\chi^{xy}$, computed in [21], is also represented (for $\mu = 0$) as a function of the temperature in Figure 2(b). As it was
pointed out in [21], the thermoelectric conductivity has a non-zero value at zero temperature implying a severe violation of the Mott relation for any value of $T$. It grows at higher $T$ in a similar way as predicted in [18] for Dirac semimetals in quantizing magnetic fields.

Inserting the thermoelectric conductivity $\chi^{xy}$ in eq. (2) we get:

$$\chi^{xy} \left( \frac{\partial \sigma^{xy}}{\partial \mu} \right)^{-1}_{\mu=E_F} = R T^2. \quad (8)$$

Figure 3 shows the ratio of the thermoelectric response function $\chi^{xy}$ and the derivative of the electric conductivity $\partial \sigma^{xy}$ at $\mu = 0$. The relation is a quadratic function of the temperature which satisfies the Mott relation except at the singular point $T = 0$. A fit of the numerical values shown as the continuum blue line in Fig. 3, gives the expression $f(\tilde{T}) = -1 - 9.29\tilde{T}^2$. Restoring the units we get, away from $T = 0$, the coefficient $R = 2.32(k_B T)^2/e$, which coincides with the standard value of $L$ to a great accuracy.

This result shows that for clean Dirac semimetals, as also happens in graphene, the $\mu = 0$ point is a singular point (the physical properties of the system at that point cannot be assumed to be the limit $\mu \to 0$ of the finite $\mu$ system) and away from it, the materials show standard Fermi liquid behaviour. It is also interesting to note that lattice effects occurring at higher energies [7] do not alter significantly the general behavior of the thermoelectric coefficients.

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