Generalization of the electrical, thermal, and thermoelectrical conductivity quanta in two and three dimensions

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The quantum Hall effect in a 2D electron system expresses a topological invariant, leading to a quantized conductivity. The thermal Hall and thermoelectric Nernst conductivities are also believed to be quantized. However, a full study of these quantities for quantum Hall systems is so far elusive. In this work, we investigate the Hall, thermal Hall, and Nernst effects analytically and numerically in 2D and 3D. We find quantized values for the Hall and thermal Hall conductivities, whereby the 3D values are the related 2D quanta scaled by a characteristic length. The Nernst conductivity is not generally quantized. Instead, an integration in energy is required to obtain a universally quantized thermoelectric quantity.

INTRODUCTION

Topological states of matter are characterized by topological invariants, which are expressed through physical quantities whose values are quantized and do not depend on the details of the system (such as its shape, size, and impurities). The best-known of these quantities is the Hall conductivity $\sigma$, which is the ratio of a transverse electrical current, generated by a longitudinal voltage under broken time-reversal symmetry (TRS) [1]. When electrons are confined to a two-dimensional (2D) system and are subjected to an external magnetic field $B$, $\sigma$ becomes exactly quantized in units of $e^2/h$, where $h$ is the Planck constant and $e$ is the elementary charge [2]. This phenomenon is called the quantum Hall effect (QHE), always requiring an external magnetic field. In its three-dimensional (3D) version, $\sigma$ is quantized in units of $e^2/h \cdot k_F^z/\pi$, where $k_F$ is the Fermi wave vector of the electrons in the direction of $B$ [3,4].

The same topological invariant is responsible for the intrinsic quantum anomalous Hall effect (QAHE) [5,10]. For 2D ferromagnetic insulators, $\sigma$ can be even quantized in units of $e^2/h$ in the absence of an external magnetic field, originating from the intrinsic magnetization of these systems. The 3D equivalent of such quantum anomalous Hall insulators are magnetic Weyl semimetals [11], which are characterized by an anomalous $\sigma$ proportional to $e^2/h \cdot k_D/(2\pi)$, where $k_D$ is the distance between the Weyl nodes [12].

Another quantity connected to topological invariants is the thermal Hall conductivity $\kappa$. It is the ratio of a heat current flowing perpendicular in response to a longitudinal temperature gradient under broken TRS [13]. In comparison to the electronic Hall effect, the thermal Hall effect also contains contributions from neutral excitations and can therefore provide additional, unique information about the topological nature of a state. In 2D electron systems subjected to external magnetic fields, the quantum thermal Hall effect (QTHE) is quantized in units of $(\pi^2 k_B^2 T)/(3h)$, where $k_B$ is the Boltzmann constant [14,19].

Analogous to $\sigma$ and $\kappa$, the thermoelectric Hall, i.e. Nernst conductivity $\alpha$, is also believed to be quantized [20,28]. It is the ratio of a transverse electrical current in response to a longitudinal temperature gradient under broken TRS. In 2D electron systems subjected to external magnetic fields, $\alpha$ is indeed quantized in units of $(ek_B)/h \cdot \ln 2$ [10]. This phenomenon is called the quantum Nernst effect (QNE).

For electronic systems, all three, the QHE, the QTHE and the QNE can be understood in terms of a Berry curvature (BC) formalism [29,34]. For 2D gapped electron systems with broken TRS, the BC formalism reveals topological invariants called Chern numbers that directly lead to a quantized $\sigma$. However, unlike the QHE, the TQHE and the QNE have so far not been investigated in 2D systems from the BC point of view. Moreover, a generalization to quantum anomalous Hall and 3D systems is also so far elusive. Therefore, it remains an open question whether the thermal Hall and the Nernst effect are as universally quantized for 2D and 3D electron systems with broken TRS as the QHE.

In this work, we study the Hall effect, the thermal Hall and the Nernst effect in the presence of a magnetic field in 2D and 3D electronic systems with both analytical and numerical methods. Moreover, we investigate the anomalous quantum effects in the Haldane model, which we expand to three dimensions. For all cases, we find that $\sigma$ and $\kappa$ are quantized in $B$. However, $\alpha$ is only quantized in 2D systems subjected to an external magnetic field and does not universally express the topological invariant of the investigated systems. Instead, its energy integral is quantized for all cases considered and seems more suitable as thermoelectric quantum than $\alpha$ itself. Our analysis reveals the quantum nature in the thermal Hall and Nernst effect as well as the influence of a weak coupling in the third dimension.

For our investigation we employ a tight-binding model on a periodic cubic lattice to ensure that the formalism for bulk systems is applicable. We use a single-band
model with a parabolic dispersion of a free electron gas for low Fermi energies

\[ H^{\text{free}}(k) = 2d + d_z - d(\cos k_x + \cos k_y) - d_z \cos k_z. \]  

(1)

This model yields the two-dimensional electron gas for \( d_z = 0 \). The third dimension can be added with a finite \( d_z \), in the following we take \( d_z = d \).

We implement an external magnetic field \( B \) along the \( z \) direction utilizing the Peierls substitution \[35\] with the vector potential \( A = (0, Bx, 0) \) leading to a modification of the hoppings as follows

\[ t_{\alpha,\beta} \rightarrow t_{\alpha,\beta}e^{i\pi B(z_{\alpha}+z_{\beta})(y_{\alpha}-y_{\beta})}. \]  

(2)

Accordingly, we choose \( B = (2\hbar)/(n ea^2) \) and increase the size of the unit cell in \( x \) direction by a factor of \( n \).

The case without an external magnetic field is described by the Haldane model \[6\]

\[ H^{\text{Haldane}}(k) = 2t_2 \cos \phi \left( \sum_{i=1}^{3} \cos (k \cdot b_i) \right) + t_1 \left( \sum_{i=1}^{3} \left[ \cos (k \cdot a_i) \sigma_1 + \sin (k \cdot a_i) \sigma_2 \right] \right) - [M - 2t_2 \sin \phi \left( \sum_{i=1}^{3} \sin (k \cdot b_i) \right)] \sigma_3 + d_z \cos (k_z) \sigma_3. \]  

(3)

Here, the last term is added to introduce a coupling in the third dimension, the two-dimensional case is achieved with \( d_z = 0 \). For a detailed discussion of the models we refer to the Supplementary Information.

**FREE ELECTRON GAS**

**2D case**

**Analytical results**

To derive quantized values for \( \sigma, \kappa, \) and \( \alpha \), we need to assume, that the Landau levels are well separated in energy for a certain temperature: \( \Delta E_{LL} \gg k_B T \). This condition can always be satisfied with low enough temperatures and large enough magnetic fields.

One can then derive the following quantizations:

\[ \sigma = \frac{e^2}{h} \sum_{n}^{occ} C_n \]  

(4)

\[ \kappa = -g_0 \sum_{n}^{occ} C_n \]  

(5)

\[ A = \int_{-\infty}^{E_F} dE \alpha(E) = -g_0 e \sum_{n}^{occ} C_n. \]  

(6)

Here, \( C_n \) is the Chern number of band \( n \), which is usually 1 for non-degenerate Landau levels, and \( g_0 = (\pi^2 k_B T)/(3\hbar) \) is the thermal conductance quantum. It is important to note, that we find \( \alpha \) itself as not quantized in general but its integral in energy \( A \) is. This can be understood from the Mott relation \[31, 32\] \( \sigma \propto \partial \alpha / \partial E \).

We can additionally include the fact, that the Landau levels have no dispersion, which means \( E_{nk} = (nek)/m_{eff} \cdot B \). In this case we find an additional quantization in the extremal peak height of the Nernst conductivity \( \alpha_{\text{ext}} \)

\[ \alpha_{\text{ext}} = -\frac{ek_B}{\hbar} \ln 2 \ C_n. \]  

(7)

In this specific case only, we find \( \alpha_{\text{ext}} \) quantized at peak heights of \( (ek_B)/\hbar \cdot \ln 2 \), consistent with observations by Checkelsky et al. \[36\].

Details of the derivations are given in the Supplementary Information.

**Numerical results**

To verify the above analytical derivation, we numerically evaluate the model in equation [4] for different sets of parameters. In the following we will
discuss one exemplarily result, for a detailed analysis we refer to the Supplementary Information.

As shown in Fig. 4(b) the introduction of a magnetic field to the 2D model creates flat Landau levels. Evaluating now $\sigma$, $\kappa$, and $\alpha$ for this case, we find a step-like behavior in both Hall, thermal Hall, and integrated Nernst conductivity $A$ (see Fig. 4(c)). Each plateau between the steps is exactly a multiple of the quantization value found in the analytical analysis and the steps occur always when a Landau level crosses the Fermi energy. $\alpha$ is always $0$ except at the Landau level crossing where it reaches the quantized value found from the analytical evaluation.

### 3D case

#### Analytical results

For the analytical evaluation of the three-dimensional free electron gas we can utilize the results already known from the 2D case and additionally carry out the integration in the third dimension. The Landau levels will stay flat for fixed $k_z$ and show a parabolic dispersion along $k_z$

$$E_{nk} = n \frac{e\hbar}{m_{eff}} B + d k_z^2.$$  \hspace{1cm} (8)

This results in a series of square-root functions added on top of each other with kinks at the energies of the Landau levels.

To simplify our results, we define a $k_0$ in the way to describe the Fermi wave vector in $z$ direction, when the second Landau level crosses the Fermi energy:

$$\frac{e\hbar}{m_e} B = d k_0^2 \rightarrow k_0 = \sqrt{\frac{\frac{e\hbar}{m_{eff}} B}{d}}.$$ \hspace{1cm} (9)

Evaluating the value a the $m-\text{th}$ kink leads to

$$\sigma = \frac{e^2}{\hbar} \frac{k_0}{\pi} \sum_{k=1}^{m} \sqrt{k}$$ \hspace{1cm} (10)

$$\kappa = -g_0 \frac{k_0}{\pi} \sum_{k=1}^{m} \sqrt{k}$$ \hspace{1cm} (11)

$$A = -g_0 e \frac{k_0}{\pi} \sum_{k=1}^{m} \sqrt{k}.$$ \hspace{1cm} (12)

Here, the three-dimensional results are given by the two-dimensional quanta scaled with $k_0/\pi$. $k_0$ is linked to the Fermi wave vector for the electron gas without a magnetic field $k_F$ via $k_0 = \sqrt{2/3} k_F$ (for details see the Supplementary Information).

For the extremal Nernst conductivity of the first peak the calculations lead to an integral that can only be treated numerically and yields

$$\alpha_{ext} \approx - \frac{e k_B}{h} \ln 2 \sqrt{\frac{k_B T}{d}} \ast 0.548.$$ \hspace{1cm} (13)

It is important to note, that this value is only dependent on the temperature $T$ and the material parameter $d$ which is linked to the effective mass. This value gives only the height of the first peak as the following peaks are always superpositions of several Landau levels.

Details of the derivations are given in the Supplementary Information.

#### Numerical results

FIG. 2. Model for the 3D free electron gas with $d = d_z = 3$ eV and $n = 30$. (a) Schematics of the 3D Quantum Hall effect. (b) Band structure without and with magnetic field $B$. Without $B$ the bands are parabolic for low energies with Fermi wave vector $k_F$, with $B$ there are flat Landau levels for constant $k_z$ and a parabolic dispersion along $k_z$ with the characteristic wave vector $k_0$. (c) Hall, thermal Hall, Nernst, and integrated Nernst conductivity with Fermi level $E_F$. The kinks occur when crossing a Landau level (dotted horizontal lines). $\sigma$, $\kappa$, and $A$ are quantized with $k_0/\pi$ as a scaling factor. The first peak of $\alpha$ is also quantized.

Similarly to the two-dimensional case, we will now discuss one specific numerical example for the 3D case and refer to the Supplementary Information for a detailed analysis.

In Fig. 2(b), the band structure of the three-dimensional electron gas is shown with and without magnetic field. The magnetic field which is
aligned along the $z$ direction leads to flat Landau levels for a fixed $k_z$ and a parabolic dispersion along $k_x$. The resulting conductivities are shown in Fig. 2 (c). Both $\sigma$, $\kappa$, and $A$ are additions of square-root functions that start at the energy of the Landau levels, leading to a characteristic kink at these energies. The value of these conductivities at the kinks is the 2D quantum scaled by $k_0/\pi \sum_{k=1}^m \sqrt{k}$ as derived in the analytical evaluation. For $\alpha$ it can be seen that the first peak reaches the predicted value and then falls off slowly to higher energies. This leads to larger peak values for the higher Landau levels because there are always the tails of the lower peaks as a background.

Haldane Model

From the free electron gas model we find that there are two quantized values for the Nernst effect so the question arises whether they are both universal. To check this, we also investigate the Haldane model given in equation (3).

2D case

3D case

FIG. 3. 2D Haldane model with $M = 0$ eV, $\phi = 0.5\pi$, $t_1 = 2$ eV, and $t_2 = 0.5$ eV. (a) Schematics of the 2D Quantum Anomalous Hall effect. (b) Band structure. (c) Hall, thermal Hall, Nernst, and integrated Nernst conductivity with Fermi level $E_F$. The dotted horizontal lines mark the global band gap. $\sigma$, $\kappa$, and $A$ are quantized in the band gap. $\alpha$ has no quantization.

FIG. 4. 3D Haldane model with $M = 0$ eV, $\phi = 0.5\pi$, $t_1 = 2$ eV, $t_2 = 0.5$ eV, and $d = 2$ eV. (a) Schematics of the 3D Quantum Anomalous Hall effect. (b) Band structure with two Weyl points. (c) Hall, thermal Hall, Nernst, and integrated Nernst conductivity with Fermi level $E_F$. $\sigma$, $\kappa$, and $A$ reach the 2D quantum scaled by the generalized Weyl point distance $k_D/(2\pi)$ at the Weyl point energy (dotted horizontal line). $\alpha$ has no quantization.

The results achieved from the analytical evaluation in equations (1), (3), and (6) are also valid for the Haldane model, because the assumption of well separated bands still holds. The result for $\alpha_{ext}$ in equation (7) is no longer valid because the assumption of flat bands is not fulfilled.

In the two-dimensional case the Haldane model shows an inverted band gap and consequently a quantized Hall conductivity for certain parameters [6]. For this study, we investigated a large parameter space and the full results are shown in the Supplementary Information. In the following we discuss one specific example.

The band structure shown in Fig. 3 (b) shows the inverted band gap of the model. It can be seen, that both conduction and valence band are indeed not flat, which is in contrast to the Landau levels discussed for the two-dimensional free electron gas. The conductivities shown in Fig. 3 (c) reach the predicted quantized value in the band gap. It can also be seen, that as a consequence of the dispersive bands $\alpha$ is stretched in energy. The exact shape is hereby determined by the dispersion. Consequently, the $\alpha_{ext}$ itself is material dependent, but $A$ remains a quantized value.
Here, $k_D = \sum^n_{i=1} c_i k_z^i$ is the generalized Weyl point distance of $n_{W_{eql}}$ Weyl points with chirality $c_i$. For one pair of points this reduces to the distance between them and leads to the result from Burkov [12]. This formulation is analogous to the first step ($m = 1$) of the three-dimensional electron gas.

In Fig. 4 (b) the band structure of a system with Weyl points is shown. Looking at the conductivities in Fig. 4 (c) there is no longer a quantized plateau because the band gap is closed at the Weyl points. Nevertheless at the Weyl point energy the values are exactly the 2D quanta scaled by $k_D/(2\pi)$ for $\sigma$, $\kappa$ and $A$. $\alpha$ itself shows no quantization.

### SUMMARY

In summary, we investigated both numerically and analytically the quantization of Hall, thermal Hall, and Nernst effect in a free electron gas model and the Haldane model for two and three dimensions. We find, that the Hall and thermal Hall effect are quantized both for an external magnetic field and an internal magnetization. To achieve a universal quantized value in a thermoelastic quantity it is necessary to integrate the Nernst conductivity in energy. Additionally, when the bands are completely flat, e.g. in Landau levels, the extremal Nernst conductivity becomes quantized. In two dimensions all these effects are quantized with natural constants, while in three dimensions these quanta are scaled by a characteristic length, namely the Fermi wave vector of the first Landau level for the free electron gas and the generalized Weyl point distance in the Haldane model. An overview of the quanta is given in Tab. I.

Perspectively, these results should also hold for the Spin Hall effect. In this case there is no transverse charge current but a transverse spin current [37]. For the Quantum Spin Hall effect (QSHE) this spin current becomes quantized [38, 39]. A possible model for the QSHE consists of two conjugated copies of the Haldane model. In this system everything shown for the Haldane model still holds, leading to similar quantizations in the QSHE and the Quantum Spin Nernst effect in both two and three dimensions.

Our results reveal for the first time a universal quantization of thermal and thermoelastic transport in two and three dimensions and show the common origin of both normal and anomalous transport effects.

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