Berry phase mediated Anomalous Thermoelectric and magnetic response in 2D Topological Insulators

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Making a long story, short...

- Brief introduction to 2D Topological Insulators

- Sleuthing for unique fingerprints of Topology

- The emergence of an Anomalous Nernst effect and Orbital Magnetization

- Original Motivation: numerous experimental observations of a Giant Nernst signal in strongly correlated electronic systems

- The conditions for a Giant Nernst Signal in Chiral states of matter

- Anomalous thermoelectricity and magnetic response in planar Topological Semiconductors
2D Topological Insulators and bulk-boundary correspondence

Definition of a Topological Insulator
A state characterized by Topologically protected edge modes

2 fundamental systems:
- Anomalous Quantum Spin Hall Insulator $\rightarrow$ Time-Reversal

\[
\begin{align*}
\text{QSH} & \\
\end{align*}
\]

- Anomalous Quantum Hall Insulator $\rightarrow$ No Time-Reversal

\[
\begin{align*}
\text{QH} & \\
\end{align*}
\]

X.-L. Qi and S.-C. Zhang, Physics Today
The Hamiltonian must include the following features:

- Spin-Orbit coupling
- Band Gap near the Γ point
- Time-reversal symmetry
BHZ Quantum Spin Hall Insulator lattice model

BHZ lattice model Hamiltonian:

\[ \mathcal{H}(\mathbf{k}) = \begin{pmatrix} \hat{\mathcal{H}}(\mathbf{k}) & 0 \\ 0 & \hat{\mathcal{H}}^*(\mathbf{-k}) \end{pmatrix}, \]

\[ \begin{pmatrix} |\mathbf{k}, m_l = 0, m_s = +\frac{1}{2} > \\ |\mathbf{k}, m_l = +1, m_s = +\frac{1}{2} > \\ |\mathbf{k}, m_l = 0, m_s = -\frac{1}{2} > \\ |\mathbf{k}, m_l = -1, m_s = -\frac{1}{2} > \end{pmatrix} \]

with

\[ \hat{\mathcal{H}}(\mathbf{k}) = \varepsilon(\mathbf{k}) + \mathbf{g}(\mathbf{k}) \cdot \tau \]

where

\[ \varepsilon(\mathbf{k}) = C - 2D(2 - \cos k_x - \cos k_y) \]

\[ \mathbf{g}(\mathbf{k}) = \begin{pmatrix} A \sin k_x, A \sin k_y, -2B \left( -\frac{M}{2B} + 2 - \cos k_x - \cos k_y \right) \end{pmatrix} \]

Band Gap at the Γ point \[ 2E(\mathbf{0}) \equiv 2|\mathbf{g}(\mathbf{0})| = 2|M| \]

For each block, the avoided band touching at the Γ point generates a finite Berry Curvature for each band in a block

\[ \Omega^z_\nu(k) = -\frac{\nu}{2} \mathbf{\hat{g}}(k) \cdot \left( \frac{\partial \mathbf{\hat{g}}(k)}{\partial k_x} \times \frac{\partial \mathbf{\hat{g}}(k)}{\partial k_y} \right) \nu = \pm \]

The Topological (Monopole) Charge that sources the Berry Curvature is equal to

\[ \tilde{N} = -\frac{1}{2\pi} \int d^2 k \ \Omega^z_-(k) = 1 \]

and provides the # of protected edge modes per block!
The finite Berry curvature acts as a $\mathbf{k}$–dependent magnetic field leading to

- **Anomalous Charge Hall effect with Hall conductivity**
  \[
  \sigma_{xy} = -\frac{e^2}{\hbar} \frac{1}{N} \sum_{\mathbf{k},\nu} \Omega^z_\nu(\mathbf{k}) n_F[E_\nu(\mathbf{k})]
  \]

  For $T = 0$ and $\mu = 0$ $\sigma_{xy} = -ne^2/h$, $n = 1$

- **Anomalous thermoelectric effect with Hall conductivity**
  \[
  \alpha_{xy} = \frac{e}{T\hbar N} \sum_{\mathbf{k},\nu} \Omega^z_\nu(\mathbf{k}) \left\{ E_\nu(\mathbf{k}) n_F[E_\nu(\mathbf{k})] + k_B T \ln \left( 1 + e^{-\beta E_\nu(\mathbf{k})} \right) \right\}
  \]

- **Finite Orbital Magnetization**
  \[
  M_{orb} = \frac{e}{\hbar N} \sum_{\mathbf{k},\nu} \Omega^z_\nu(\mathbf{k}) \left\{ E(\mathbf{k}) n_F[E_\nu(\mathbf{k})] + k_B T \ln \left( 1 + e^{-\beta E_\nu(\mathbf{k})} \right) \right\}
  \]
Berry-Curvature-originating fingerprints, for detecting Topological Order in 2D

Anomalous Quantum Hall state: **Single block Hamiltonian**!
- Anomalous Hall effect
- Anomalous charge Thermoelectric effect
- Finite Orbital Magnetization

Anomalous Quantum Spin Hall state: **Two block Hamiltonian with opposite Berry curvature per block**!
- Anomalous Spin Hall effect
- Anomalous Spin Thermoelectric effect
- Finite additional Zeeman Magnetization **due to Orbital effects**!
Thermoelectric Transport and Nernst Signal

- Constitutive relations for *thermoelectric charge transport*

\[
\begin{align*}
J_x &= \sigma_{xx} E_x + \sigma_{xy} E_y + \alpha_{xx} (-\partial_x T) \\
J_y &= \sigma_{yx} E_x + \sigma_{yy} E_y + \alpha_{yx} (-\partial_x T)
\end{align*}
\]

with \( J \equiv \text{charge current}, \ E \equiv \text{electric field}, \ T \equiv \text{temperature} \)

- *Thermopower* \( S \Rightarrow \text{longitudinal} \) voltage appearing for \( J = 0 \)

- *Nernst signal* \( N \Rightarrow \text{transverse} \) voltage appearing for \( J = 0 \)

\[
S \equiv \frac{\mathcal{E}_x}{\partial_x T} \quad \text{and} \quad N \equiv \frac{\mathcal{E}_y}{-\partial_x T}
\]

**Anomalous N**

\[ \to \mathcal{B}_z = 0 \]
Quasiparticle and Vortex sources of a Nernst signal

**Quasiparticles**

1. **Transverse velocity due to the Lorentz force** ⇒ $N \sim B_z$

2. Nernst signal takes both signs depending on Doping

3. Nernst signal strongly linear in Temperature

4. **Single band metals show a tiny Nernst signal** $\sim nV/K$ due to Sonheimer cancellation


**Superconducting Vortices**

1. **Normal Core Entropy + Vortex attached Flux** ⇒ $\alpha_{xy} \neq 0$

   ⇒ $N \sim B_z$, B. D. Josephson, Physics Letters 16, 242 (1965)

2. **Only Positive** Nernst signal !!!!

3. Nernst signal non-linear in Temperature
Chirality driven Nernst signal

Chirality \equiv \text{Finite Angular Momentum}

1. Violation of Time-Reversal \Rightarrow \sigma_{xy}(B_z = 0) \neq 0 \text{ and } \alpha_{xy}(B_z = 0) \neq 0 \Rightarrow \text{Anomalous Hall + Nernst Effects!}

2. “Magnetic-field” in k-space: the Berry curvature \Omega_z(k).

3. The Nernst signal takes both signs !!!!

4. Large Fermi-Surface \Rightarrow N \text{ linear in Temperature}

Examples

- \text{CuCr}_2\text{Se}_4-x\text{Br}_x: \text{Spinel Ferromagnet + Spin-Orbit coupling}

- Heavily-Doped Chiral \text{d}_{xy} + \text{id}_{x^2-y^2} \text{ Density Wave}

But what happens in the Strongly Insulating limit??????

Chirality Induced Tilted-Hill Giant Nernst Signal:
Giant Tilted-Hill Nernst signal in High-Tc cuprates

- Giant N in Pseudogap + Superconducting regimes
- Tilted-Hill (peaked) temperature profile
- Positive Nernst signal
- Enhanced Diamagnetism in the pseudogap phase
- Diamagnetism scales with the Nernst signal

Yayu Wang, Lu Li, and N. P. Ong, PRB 73, 024510 (2006)
Giant Tilted-Hill Nernst signal in the heavy fermion compound URu$_2$Si$_2$

- The non-SC order in the phase diagram $\equiv$ “Hidden Order” (HO)
- Giant N in the Hidden Order
- Tilted-Hill temperature profile
- No Diamagnetism!
- For low $T$, the HO condenses in a SC state, possibly Topological

Y. S. Oh et al, PRL 98, 016401 (2007)

Chiral $d_{xy} + id_{x^2-y^2}$ Density Wave

- Chiral D-Density waves have been recently proposed for understanding the Pseudogap regime in the cuprates (PK and G. Varelogiannis 2008 & S. Tewari et al. 2008) and the Hidden Order (PK, A. Aperis and G. Varelogiannis 2010)

- The very-same interactions promoting unconventional superconductivity, also favour Chiral Density Wave formation

- Half-filled single band square lattice model:

$$\mathcal{H}_0 = -2t \sum_k (\cos k_x + \cos k_y) c_{k\uparrow} c_k$$

- Enhanced tendency towards an Insulating Chiral D-Density Wave due to perfect nesting

- Formation of a Topological Insulating Condensate
Pairing interactions and Mean-field decoupling

- Intersite extended Hubbard interactions up to n.n.n.

\[ \mathcal{H}_{\text{int}} = \sum_{\langle\langle i,j\rangle\rangle} \left( V_{ij} n_i n_j + J_{ij} \vec{S}_i \cdot \vec{S}_j \right) \]

- Driving effective interaction \( \sim \sum_{k,k'} V_{k,k'} c_k^\dagger c_{k+Q} c_{k'}^\dagger + Q c_{k'} \)

- Chiral d-density wave "Anomalous" Terms \( \Delta(k) c_k^\dagger c_{k+Q} + h.c. \)

**Chiral D-Density Wave Order Parameter:**

\[ \Delta(k) \sim \sum_{k'} V_{k,k'} <c_{k'}^\dagger + Q c_{k'}> \Rightarrow \]

\[ \Delta(k) = \Delta_1 \sin k_x \sin k_y - i\Delta_2 (\cos k_x - \cos k_y) \]
Mean-field Hamiltonian of a chiral d-density wave

- Nambu isospinor $\Psi_k^\dagger = (c_k^\dagger \ c_{k+Q}^\dagger)$, $k \in$ reduced B.Z.

- We obtain a pseudospin-$\frac{1}{2}$ system for each $k$-point

$$\mathcal{H}(k) = \begin{pmatrix} \varepsilon(k) + g_3(k) & g_1(k) - ig_2(k) \\ g_1(k) + ig_2(k) & \varepsilon(k) - g_3(k) \end{pmatrix} = \varepsilon(k)I_\tau + g(k) \cdot \tau$$

- $g_1(k) = \Delta_1 \sin k_x \sin k_y$, $g_2(k) = \Delta_2 (\cos k_x - \cos k_y)$,

- $g_3(k) = -2t(\cos k_x + \cos k_y)$ and $\varepsilon(k) = -\mu$.

- 2-Band Energy Spectrum: $\nu = \pm \rightarrow E_{\nu}(k) = \varepsilon(k) + \nu|g(k)|$
Steps for calculating the Tilted-Hill Giant Nernst signal

1. We obtain self-consistently the Chiral Order Parameter

PK and G. Varelogiannis, PRB 80, 212401 (2009)

2. Anomalous thermoelectric Hall conductivity

\[
\alpha_{xy} = \frac{e}{T \hbar N} \sum_{\mathbf{k}, \nu} \Omega^Z_\nu (\mathbf{k}) \left\{ E_\nu (\mathbf{k}) n_F [E_\nu (\mathbf{k})] + k_B T \ln \left( 1 + e^{-\beta E_\nu (\mathbf{k})} \right) \right\}
\]

3. \( \sigma_{xx} \) and \( \alpha_{xx} \) in the Boltzmann approximation

\[
\sigma_{xx} = -\frac{e^2}{\hbar} \frac{1}{N} \sum_{\mathbf{k}, \nu} n'_F [E_\nu (\mathbf{k})] \frac{\tau_\nu (\mathbf{k})}{\hbar} \left( \frac{\partial E_\nu (\mathbf{k})}{\partial k_x} \right)^2
\]

\[
\alpha_{xx} = +\frac{ek_B}{\hbar} \frac{1}{N} \sum_{\mathbf{k}, \nu} n'_F [E_\nu (\mathbf{k})] \frac{\tau_\nu (\mathbf{k})}{\hbar} \left( \frac{\partial E_\nu (\mathbf{k})}{\partial k_x} \right)^2 \frac{E_\nu (\mathbf{k})}{k_B T}
\]

4. We ignore quasiparticle Hall conductivities

5. For finite \( B_z \neq 0 \), \( E_\nu (\mathbf{k}) \), \( \tau_\nu (\mathbf{k}) \), DOS get modified

D. Xiao, M.-C. Chang and Q. Niu, Rev. Mod. Phys. 82, 1959 (2010)
Mechanism of the Chirality Induced Tilted-Hill Giant Nernst signal

- For low temperatures, the strongly insulating character leads to the condition $\sigma_{xx} \ll \sigma_{xy}$ providing $S \simeq \alpha_{xy}/\sigma_{xy}$ and $N \simeq -\alpha_{xx}/\sigma_{xy}$.

- **A Thermoelectric crossing point** emerges at $\sigma_{xx} = \sigma_{xy}$, where $S = N$.

- After the crossing, $\sigma_{xx} \gg \sigma_{xy}$, provides $S \simeq \alpha_{xx}/\sigma_{xx}$, $N \simeq \alpha_{xy}/\sigma_{xx}$.

- **Crucial**: $N = S$. The usually high values of $S$, unavoidably lead to an enhancement of the Nernst voltage.

\[
S = \frac{\alpha_{xx}\sigma_{yy} + \alpha_{xy}\sigma_{xy}}{\sigma_{xx}\sigma_{yy} + \sigma_{xy}^2}
\]

\[
N = \frac{\sigma_{xx}\alpha_{xy} - \alpha_{xx}\sigma_{xy}}{\sigma_{xx}\sigma_{yy} + \sigma_{xy}^2}
\]

($t = 250\text{meV}$, $\mu = 0$, $a = 5\text{Å}$, $d_{x^2-y^2} = 53\text{meV}$, $\tau = 10^{-13}\text{s}$, $B_z = 5\text{T}$ and $d_{xy} \simeq 22\text{meV}$)

Properties of the Novel Anomalous Nernst Effect

- Emergence of a Thermoelectric Point
- Around the vicinity of this point, the Nernst signal exhibits a peak due to the crossover behaviour, leading to the *Tilted-Hill* profile
- The Nernst signal may be inverted by tuning the chemical potential or the doping of the sample

![Graph showing Nernst signal vs. temperature (T(K)) for different chemical potentials (μ): μ=+3meV, μ=+1meV, μ=−0.9meV, μ=−2.9meV, μ=−4.8meV.](image-url)
To engineer the long-sought Quantum Anomalous Hall state we can start from

- either a planar Anomalous Quantum Spin Hall state or
- by the surface of a $\mathcal{T}$-invariant 3D Topological Insulator which is described by a helical-liquid

$$\mathcal{H}(\mathbf{k}) = -\mu + k_y \sigma_x - k_x \sigma_y .$$

In both case $\mathcal{T}$-invariance must become violated via the following routes

1. magnetic impurities
2. perpendicular to the surface Zeeman field
3. Ferromagnetic coating

$\mathcal{T}$-violation leads to an effective BHZ single block model
Results on the Anomalous Nernst signal in the Anomalous Quantum Hall state

- We observe that the Anomalous Nernst signal becomes giant of the order $mV/K$
- There exist a thermoelectric crossing point where $N = |S|$. 
- The Nernst response may be directly tuned by the doping of the system

\[ M = -1.2\, \text{meV}, \quad \tau = 10^{-13}\, \text{s}, \quad a = 0.65\, \text{nm} \]
The additional contribution to the Zeeman magnetization can be in principle detected due to the

- temperature dependence that it demonstrates (although weak)
- its doping dependence that controls its sign!

![Graph showing the temperature dependence of orbital magnetization for different chemical potentials. The y-axis represents the orbital magnetization in units of \( \mu_B \), and the x-axis represents temperature in Kelvin. Three lines are shown, each labeled with the chemical potential: C–\( \mu \) = -52.6 meV, C–\( \mu \) = -26.3 meV, and C–\( \mu \) = 0 meV. The graph demonstrates how the magnetization changes with temperature for each case.]
We demonstrated a novel source of Giant Thermoelectricity that is dictated by a Tilted-Hill temperature profile and originates from a well insulated Chiral state in the case of strongly correlated systems.

The Anomalous Quantum Hall state could be detected due to a giant Nernst signal and an accompanying Thermoelectric crossing point.

The Berry Curvature induced Zeeman magnetization constitutes a magnetofingerprint for the detection of an Anomalous Quantum Spin Hall state through its temperature and doping dependence.
Thanks for your attention!