Transport Experiments on 3D Topological insulators

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1. Transport in non-metallic Bi$_2$Se$_3$ and Bi$_2$Te$_3$
2. A TI with very large bulk $\rho$ – Bi$_2$Te$_2$Se
3. SdH oscillations to 45 Tesla – Evidence for $\frac{1}{2}$ shift from Dirac Spectrum
4. Is there a Zeeman induced shift at $n = 0$?
5. Hydrostatic pressure – bulk band structure

Support from
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DARPA
ARO
In Bi$_2$Se$_3$ and Bi$_2$Te$_3$

- Only 1 surface state present
- Massless Dirac spectrum
- Large gaps -- 300 and 200 meV
Difficult to resolve surface states by transport

Onset of non-metallic behavior ~ 130 K

Bulk SdH oscillations seen in both n-type and p-type samples

Non-metallic samples show no discernible SdH (disorder from Ca dopants)

Checkelsky et al., PRL '09
Magnetoresistance of gapped Bi2Se3

Giant, quasi-periodic, retraceable conductance fluctuations

Checkelsky et al., PRL ‘09

Logarithmic anomaly

Sample G4

Graphs showing the magnetoresistance of Bi2Se3 with logarithmic anomaly.
Shubnikov de Haas Oscillations in non-metallic Bi$_2$Te$_3$

Qu, NPO et al. *Science*, 2010

Non-metallic crystals

Metallic crystal

SdH oscillations in Hall conductivity
2D vs 3D Shubnikov de Haas period in bulk Bi$_2$Te$_3$

Non-metallic sample

Metallic sample

Qu, NPO et al. Science 2010

SdH period $S_F$ scales as $\cos \theta$

Hence, 2D

Period $S_F$ deviates from 2D

Hence, 3D

ellipsoid
Temperature dependence of Shubnikov de Haas amplitude

Qu, NPO et al. 2010

SdH amplitude decreases with $T$.

For massless Dirac states, we fit to

$$\Delta \sigma(H, T) \sim \frac{\lambda}{\sinh(\lambda)} e^{-D}$$

$$m_c = \frac{E}{v_F^2}$$

$$\lambda = \frac{2\pi^2 k_B T}{h \omega_c}$$

$$D = \frac{2\pi^2 k_B T_D}{h \omega_c}$$

Fits yield

- $m_c = 0.1 \ m_0$
- $v_F = 3.7 -- 4.1 \times 10^5 \text{ m/s}$
- (ARPES gets $4 \times 10^5$).
1. (Panel A) Hall conductivity $\sigma_{xy}$ shows a “resonance” anomaly in weak $H$

2. (Panel B) After subtracting bulk contribution, the resonance is the isolated surface Hall conductivity $G_{xy}$. Peak position yield mobility $\mu$ ($\sim 9,000$ cm$^2$/Vs) and peak height yields metallicity $k_F\ell = 80$.

Panel B is a “snap shot” that gives mobility and $k_F\ell$ by inspection.
Fit (semiclassical)

\[ \sigma_{xy} = \sigma^b_{xy} + G_{xy} / t \]

\[ \sigma^b_{xy} = n_b e \mu_b \frac{\mu_B H}{[1 + (\mu_B H)^2]} \]

\[ G_{xy} = \frac{e^2}{h} k_F \ell \frac{\mu_s H}{[1 + (\mu_s H)^2]} \]

\[ \mu_s = \frac{e \ell}{\hbar k_F} \]

\[ \ell = 240 \text{ nm} \quad \mu_s = 8,000 \text{ cm}^2/\text{Vs} \]

- Good agreement with Dingle analysis & 2D massless Dirac state.

- Numbers rule out \( G_{xy} \) as 3D bulk term.
## Comparison of transport parameters

<table>
<thead>
<tr>
<th>Material</th>
<th>$R_{\text{obs}}$ (Ω)</th>
<th>$\rho_b$ (mΩ cm)</th>
<th>$\mu_s$ (cm$^2$/Vs)</th>
<th>$k_F l$</th>
<th>$G_s/G_{\text{bulk}}$</th>
<th>$\mu_s/\mu_b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bi$_2$Se$_3$ (Ca)</td>
<td>0.01</td>
<td>30-80</td>
<td>&lt; 200</td>
<td>?</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>Bi$_2$Te$_3$</td>
<td>0.005</td>
<td>4-12</td>
<td>10,000</td>
<td>100</td>
<td>0.03</td>
<td>12</td>
</tr>
<tr>
<td>Bi$_2$Te$_2$Se</td>
<td>300-400</td>
<td>6,000</td>
<td>2,800</td>
<td>40</td>
<td>~1</td>
<td>60</td>
</tr>
</tbody>
</table>
Topological Insulator with sharply reduced bulk cond. --- Bi$_2$Te$_2$Se

- Xiong, Cava, NPO
  - *cond-mat/1011.1315*

- Also,
  - Y. Ando et al., PRB ‘11

**Bulk mobility** $\mu_b \sim 50$ cm$^2$/Vs

**Bulk carrier density** $n_b \sim 2.6 \times 10^{16}$ cm$^{-3}$
Band Structure of Bi$_2$Te$_2$Se

Obtain $m^*$ and $v_F$ from $T$ dependence of amplitude, $\text{Bi}_2\text{Te}_2\text{Se}$

Fit yields
$m^* = 0.089$
$v_F = 6 \times 10^5 \text{ m/s}$
Determine mobility and mfp from field dependence

Require 2 terms with different $k_F$'s (differ by 2.5%)

$m^* = 0.089$

$T_D = 7.2$ K

$\ell = 100$ nm

$k_F \ell = 49$

$\mu_s = 2,800$ cm$^2$/Vs

$\mu_s/\mu_b = 60!$

\[
\frac{\Delta \sigma}{\sigma} = \sqrt{\frac{\hbar \omega_c}{2E_F}} \frac{\lambda}{\sinh(\lambda)} e^{-D} \cos\left(\frac{2\pi E_F}{\hbar \omega_c} + \frac{\pi}{4}\right)
\]

$\lambda = 2\pi^2 \frac{k_B T}{\hbar \omega_c}$

$D = 2\pi^2 \frac{k_B T_D}{\hbar \omega_c}$
½ shift expected in Index Plot in Dirac spectrum

Resolution is insufficient. Need \( B > 14 \) Tesla

- **Indexing scheme**
  - **Minima** of \( G_{xx} \) obs. when \( \mu \) lies between LL
  - \( B_n \) (min) aligns with index \( n \)
  - Schrödinger spectrum ➔ intercept \( \gamma \) is 0 (mod 1)
  - Dirac spectrum ➔ Intercept \( \gamma \) is \( -\frac{1}{2} \) (mod 1)
$\text{Bi}_2\text{Te}_2\text{Se}$

The graph shows the dependence of $d\rho_{yx}/dB$ (arb. units) on $1/B(T^{-1})$. The data is presented for different temperatures: 0.35 K, 1.5 K, 4.4 K, 7 K, and 10 K. There are vertical dashed lines at $1/B(T^{-1})$ values of 0.0835, 0.0980, 0.1109, 0.1245, and 0.1382.
Amplitude of SdH oscillations is 17% of total conductance

*Derivatives* not needed to resolve SdH oscillations

Bulk resistivity $\rho_b = 4 - 8 \ \Omega \text{cm} \ (\sim 4 \text{ K})$

Oscillations seen in both $G_{xx}$ and $G_{xy}$
Isolate SdH oscill terms $\Delta G$, $\Delta G_{xy}$

Largest oscillations seen to date in Bi based TI’s

Peak-to-peak amplitudes

$\sim \frac{e^2}{h}$ in $\Delta G_{xy}$

$\sim 4\frac{e^2}{h}$ in $\Delta G$

Fit to Lifshitz expression yields

$\mu = 3,200 \text{ cm}^2/\text{Vs}$
The $g$-factor of topological states

Competition between Rashba and Zeeman terms

\[ \pi = p + eA \]

\[ H = v_F (\sigma^x \pi_y - \sigma^y \pi_x) - \left(\frac{g \mu_B}{2}\right) B \cdot \sigma \]

Rashba

\[ H = v_F \sqrt{2\hbar eB} \begin{bmatrix} 0 & b \\ b^* & 0 \end{bmatrix} - \frac{g \mu_B B}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \]

Zeeman

In $n = 0$ level, only Zeeman term remains

\[ E_n = \pm \sqrt{2\hbar v_F^2 eB + (g \mu_B B / 2)^2} \]

R. Mong and J. Moore, unpub.
Seradjeh, Wu, Phillips. PRL 2009

- In $\text{Bi}_2\text{Te}_2\text{Se}$, chemical potential $\zeta$ is fixed (rather than $n_s$)
- Large $g$ causes deviation in index plot
Limiting behavior as \( n \to 0 \)

Intercept (\( 1/B \to 0 \))
\[ \gamma = -0.40 \to -0.55 \]

Transport evidence for Dirac spectrum

At 40 T (\( n = \frac{1}{2} \)), we have (\( \frac{1}{2} + \frac{1}{2} \)) LLs below \( \mu \)

No evidence for Zeeman shift
Quantum Oscillations in Bi$_2$Te$_2$Se (Sample 2)

Oscillation amplitude 10 times weaker than in 1.

Index plot intercept
\[ \gamma = -0.45 \]

Also supports Dirac spectrum
Effect of hydrostatic pressure on $\text{Bi}_2\text{Te}_2\text{Se}$

Yongkang Luo, Stephen Rowley et al.

Progress in understanding bulk band structure of $\text{Bi}_2\text{Te}_2\text{Se}$

**Issues:**

Where is the gap in transport?

Where is the carrier no. activation?

Why does Hall change sign vs. T?

Large thermopower and ZT in Bi-based semimetals?
Effect of pressure on Hall coefficient in Bi$_2$Te$_2$Se

![Graphs showing the effect of pressure on Hall coefficient](image)
Model of band structure inferred from transport in Bi$_2$Te$_2$Se

By simultaneous fits to $\sigma_{xx}$ and $\sigma_{xy}$

Thermal activation of holes to valence band (gap $\Delta \sim 50$ mV)
Chemical potential $\mu$ increases with $T$ as $T^2$
Bulk mobility $\mu_b \sim 1/T$
Gap very sensitive to hydro. pressure
Best fit yields $\Delta = 50$ mV, $m_h = 0.18$ at ambient pressure.
Summary

Surface topological states cleanly observed by SdH oscillations

Surface mobilities are high, 12x bulk mob. (Bi$_2$Te$_3$) to 60x (Bi$_2$Te$_2$Se)

Ratio of $G_s$ to $G_b$ is ~ 1 in Bi$_2$Te$_2$Se

Quantum oscil. obs. to 45 Tesla resolves ½-shift from Dirac spectrum

Oscill. amplitude in $G_{xy}$ is $\sim e^2/h$

Bulk transport ($\sigma_{xx}$ and $\sigma_{xy}$ vs. $T$) well-described by gap ~ 50 mV; $T$-dependent chemical potential

20 kbar pressure closes gap
In non-metallic crystals, the surface mobility ($10,000 \text{ cm}^2/\text{Vs}$) is $>10$ times higher than in the bulk.

Consequence $\rightarrow$ weak-field “resonance” in the Hall conductivity.

from deflection of high-mobility carriers in weak $H$

In a 1 kG field, surface electrons (blue) display large Hall signal, but heavy bulk holes (red) are barely deflected.
Fixed fixed carrier density $n_s$, or fixed chemical potential $\zeta$?

Surface charging energy $Q^2/2C$

We assume fixed $\zeta$ (anchored to bulk $\zeta_b$)
Tune chemical potential in $\text{Bi}_2\text{Se}_3$ by back gate

Flat band case

Chemical potential $\mu$ in the cond. band

Chemical potential moves inside gap if $d$ is thin enough
We fitted Hall conductivity with

$$\sigma_{xy} = \sigma_{bxy} + \frac{G_{xy}}{t}$$

**Why is $G_{xy}$ a 2D term?**

Let’s assume it is a 3D electron pocket, and write

$$\frac{G_{xy}}{t} \Rightarrow ? \quad n' e \mu \frac{\mu H}{[1 + (\mu H)^2]}$$

Since $\mu = 10,000 \text{ cm}^2/\text{Vs}$, we find $n' = 1.4 \times 10^{14} \text{ cm}^{-3}$ with $k_F' = 1.6 \times 10^{-3} \text{ Å}^{-1}$

This differs from $k_F$ observed in SdH by a factor of 19.

i.e. disagrees with SdH period by 360.
4. SdH at ambient pressure

Shubnikov-de Hass oscillation is observed, both in MR and Hall channel, and will persist to higher than 30 K.
\[
\frac{\Delta \sigma_{xx}}{\sigma_{xx}} \propto A(1/B) \exp\left(-\frac{\pi m_c}{\tau e} \frac{1}{B}\right) \cos\left(\frac{\hbar S_F}{e} \frac{1}{B} + \gamma\right)
\]

\[k_F = 0.0471 \text{ A}^{-1}\]
\[\gamma = -0.342 \pi\]
\[\frac{\pi m_c}{\tau e} = 52.77\]

Lifshitz expression fit leads to \(k_F=0.0471 \text{ A}^{-1}\), which is close to as grown BTS. But the temperature dependence of oscillation amplitude is hard to fit simply with

\[\frac{\lambda}{\sinh(\lambda)}\]

Coincidently, the amplitude starts to decrease fast when \(T>15\text{K}\), which is consistent with \(R(T)\) curve.
We observed a new set of quantum oscillation under low pressure.
These new peaks are observed at different temperatures at the same position, and will freeze out at higher temperature, all these suggests that this phenomenon is intrinsic.

We subtract a smooth background and get this profile. We can confirm several prominent features:

1. The new set of oscillation has a period that is very close to the original one, which indicates it has a similar k_F.
2. The new set of oscillation is un-resolvable at low field, but becomes very robust at high field, and will overwhelms the original oscillations. This means the new set of oscillation has a much smaller mobility.
Considering the band bending model, $\sigma_{xy}$ can be fit as:

$$\sigma_{xy} = A \frac{\mu_s^2 B}{1 + \mu_s^2 B^2} + C \frac{\mu_b^2 B}{1 + \mu_b^2 B^2}$$
\[ \sigma_{xy} = A \frac{\mu_s^2 B}{1 + \mu_s^2 B^2} + C \frac{\mu_b^2 B}{1 + \mu_b^2 B^2} \]

The first term is the surface, while the second is band-bending effect induced bulk contribution. A and C are proportional to the corresponding carrier density, respectively.

<table>
<thead>
<tr>
<th>P (kbar)</th>
<th>A</th>
<th>C</th>
<th>(\mu_s) (cm²/Vs)</th>
<th>(\mu_b) (cm²/Vs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>-23.8</td>
<td>-287</td>
<td>2340</td>
<td>520</td>
</tr>
<tr>
<td>0.4</td>
<td>-10.8</td>
<td>-1255.9</td>
<td>1710</td>
<td>286</td>
</tr>
<tr>
<td>0.9</td>
<td>-4.4</td>
<td>-1417.6</td>
<td>1948</td>
<td>249</td>
</tr>
</tbody>
</table>

Now we can get: \(l = 7.27 \times 10^{-8} \text{ m}\), \(k_F l = 34\)

This fit supports our band bending assumption:

(1) Tiny pressure causes band bending effect, which is responsible for the new set of quantum oscillation.

(2) Larger pressure causes more obvious band bending effect, and more contribution from band bending effect in \(\sigma_{xy}\), because the mobility is much lower than the surface, it makes the \(\sigma_{xy} \sim B\) more linear.