OVERVIEW

• What are topological insulators and Dirac semimetals?

• Quantum transport and magnetic properties (quantum oscillations).

• Synthesis

• Some concrete materials and measurements.
TOPOLOGICAL INSULATORS (TI)

Topological insulator (TI)

Quantum state characterized by topological invariant (nontrivial).

There is an energy gap.

Defined over the wave functions (that give the energy gap)

- Invariant under adiabatic change of Hamiltonian.
- The same as long as there is a gap!

- Closing of the energy gap at the boundary of topological and normal insulator (vacuum)

  conductive edge/surface
TOPOLOGICAL INSULATORS

- Examples of TI and topological invariant?

\( Z_2 \) TI (TRS & IS)

Quantum Hall effect

\[ \sigma_{xy} = n \frac{e^2}{h}, \quad n \in N \]

Edge states

\( n \rightarrow \) topological invariant

(TRS, 2D)

Chern number or TKNN

\( \nu = 0,1 \rightarrow Z_2 \) topological invariant

Time reversal operator: \( \Theta^2 = -1 \)

Nontrivial topological invariant if there is a band inversion at some \( \lambda \)!

Topological crystalline insulator

\( \nu = 0 \), topological invariant is not determined by TRS but with crystal symmetries (mirror symmetry).

\[ M^2 = -1 \]

\( \nu \)

(Chern number or TKNN)

TRS, 2D

Atomic orbitals

\( \xi_{2\pi} \)

parity

\( \nu \)

Time reversal operator:

\( \Theta^2 = -1 \)

\( M^2 = -1 \)

Topological crystalline insulator

\( \nu = 0,1 \rightarrow Z_2 \) topological invariant

3D: \( \nu_0, \nu_1, \nu_2, \nu_3 \)

SOC – spin orbit coupling
TOPOLOGICAL INSULATORs

- Edge/surface states properties.

Dirac dispersion in low-energy excitations ➞ high mobility!

Spin-momentum locking ➞ forbidden backscattering!
DIRAC SEMIMETALS

Dirac dispersion in 3D!

2D – graphene: $\hat{H}(\mathbf{k}) = v(k_x \sigma_x + k_y \sigma_y) \rightarrow$ SOC $\sim \sigma_z$ opens the gap.

3D: $\hat{H}(\mathbf{k}) = v_{ij} k_i \sigma_j, \quad j = x, y, z \rightarrow$ Robust against perturbations!
Dirac semimetals come in two topological classes too.

Consequence of topological phase transition NI – TI.

Intrinsic as a result of additional symmetries (rotational symmetry).
• Topological insulators $\rightarrow$ 2D Dirac dispersion.
• Dirac semimetals $\rightarrow$ 3D Dirac dispersion.

Possibility for investigating Dirac’s fermion physics!

Evidence of Dirac fermions?
QUANTUM OSCILLATIONS

- Electrons in strong B-field \( \rightarrow \) Landau levels.

For Dirac dispersion \( E_{\pm}(k) = \pm v_f k \)

\[
E_{\pm}(N) = \pm \sqrt{\left(2e\hbar v_f^2 B / c \right)N}
\]

Periodic behavior of DOS.

Oscillations of physical quantities in \( 1/B \! \! \! \! \! \slash \)!

\[ E = \left( N + \frac{1}{2} \hbar \omega \right) + \frac{\hbar^2 k_z^2}{2m} \rightarrow \text{for } E(k) = \frac{\hbar^2 k_z^2}{2m} \]

\[ M \rightarrow \text{de Haas van Alphen oscillations.} \]
\[ \sigma \rightarrow \text{Shubnikov de Haas oscillations.} \]

Downloaded from J. Phy. Soc. Jap. 82, 102001 (2013).
QUANTUM OSCILLATIONS

• de Haas van Alphen and Shubnikov de Haas oscillations (for 3D)

\[ \Delta M = A R_T R_D R_s \sin 2\pi \left( \frac{F}{B} - \frac{1}{2} - \frac{1}{8} + \beta \right) \]

\[ \Delta \sigma_{xx} = A R_T R_D R_s \cos 2\pi \left( \frac{F}{B} - \frac{1}{2} - \frac{1}{8} + \beta \right) \]

\[ 2\pi \beta = \gamma \quad \text{Berry phase!} \]

\[ \gamma = i \frac{e}{h} \int \vec{k} \left| \psi(\vec{k}) \right\rangle \left\langle \nabla_k \psi(\vec{k}) \right| \]

For Dirac fermions

\[ \gamma = \pi \]

Informations about carrier density and Fermi surface shape.

Effective mass

Quantum scattering time

\[ \alpha = 14.69 \frac{m}{m_0} TK^{-1} \]

\[ R_T = \frac{\alpha T}{B \sinh(\alpha T/B)} \]

\[ R_D = e^{\alpha T/B} \]

\[ R_s = \cos \left( \frac{\pi g m}{2 m_0} \right) \]

\[ F = \frac{\hbar}{2e} k_f^2 \]

\[ T_D = \frac{\hbar}{2\pi k_f} \]
SYNTHESIS

• Aim: high quality monocrystal samples.
• The fewer impurities and defects minimize the influence of bulk states and increase mobility.

Sealing the quartz tube.

High vacuum in ampoule
• clean atmosphere
• volatile elements

Material in vacuum sealed quartz ampoule (vacuum $\sim 10^{-6}$ mbar)
SYNTHESIS

- Modified Bridgman method.

- (Chemical) vapor deposition.

Temperature gradient is achieved by two-zone tube furnaces.

Synthesis parameters:
- temperature, gradient, heating/cooling rate, growth time,
- amount and shape of material, ampoule dimensions.

Optimization of parameters!
SYNTHESIS

Results of synthesis:

- BiSbTeSe$_2$
- PbSnSe
- SnTe
- Cd$_3$As$_2$
- TaP
SAMPLE PREPARATION

• For transport measurements good contacts are crucial (~ Ω).

Samples of Cd₃As₂ with contacts.

Spot welding
PbSnSe

- \( \text{Pb}_{1-x}\text{Sn}_x\text{Se} \) is a topological crystalline insulator for \( x > 0.23 \).
- Known for ages: energy gap depends on the \( T \) and \( x \).
  - Topological phase transition with \( T \) or \( x \).
- What happens at the transition point? (\( x \approx 0.18 \))
PbSnSe

- Magnetization (SQUID) and magnetoresistance measurements in Pb$_{0.82}$Sn$_{0.18}$Se.
PbSnSe

- By subtracting the background we get a pure oscillatory part.
PbSnSe

• How to get physical values from quantum oscillations?

\[ \Delta M = A R_T R_D R_s \sin \left[ 2\pi \left( \frac{F}{B} - \frac{1}{2} \frac{1}{8} + \beta \right) \right] \]

\[ \Delta \sigma_{xx} = A R_T R_D R_s \cos \left[ 2\pi \left( \frac{F}{B} - \frac{1}{2} \frac{1}{8} + \beta \right) \right] \]

\[ R_T = \frac{\alpha T}{B} \frac{1}{\sinh \left( \frac{\alpha T}{B} \right)} \]

\[ R_D = e^{\frac{-\alpha T}{B}} \]
**Cd$_3$As$_2$**

- Cd$_3$As$_2$ is an intrinsic (nontrivial) Dirac semimetal.
- Very stable material, except toxicity ideal for application and experiment.
- High mobility $\sim 10^6 \text{cm}^2\text{V}^{-1}\text{s}^{-1}$.
- A pair of Dirac points in the direction of rotational symmetry axis ($k_z$).
- Anisotropy of Fermi surface? Different frequencies for different direction of magnetic field.

Different frequencies for different direction of magnetic field.

3D Dirac semimetal Cd$_3$As$_2$
Cd$_3$As$_2$

- Magnetization and magnetoresistance are measured.

\[ F = 60 \, \text{T} \]

B in ab plane.

B perpendicular to ab plane.

Superposition of frequencies.
OTHER MATERIALS

- Other materials we have successfully synthesized:

- **TaP** → Weyl semimetal candidate.

  ![Graph showing quantum oscillations for TaP](image)

  Successfully observed quantum oscillations.

- **BiSbTe$_2$S** → topological insulator.

  ![Graph showing typical semiconducting behavior](image)

  Metallic behavior because of surface states.

  Typical semiconducting behavior.
CONCLUSION

• Topological insulators.
  • symmetry protected surface states → spin locking and robustness at nonmagnetic impurities.

• Dirac semimetals.
  • 3D analogue of graphene. Symmetry protected Dirac points.

• The idea is to synthesize (determination of synthesis parameters) and characterize the obtained materials.

• Examine the consequences of the Dirac nature of carriers in magnetization and transport.

→ An insight into the physics of Dirac’s fermions.