Topological Materials Predicted by OpenMX

Hongming Weng (翁红明)

Institute of Physics,
Chinese Academy of Sciences

Nov. 23-25@KAIST, Daejeon
2016 Nobel Prize in Physics

David J. Thouless
University of Washington, Seattle, WA, USA

F. Duncan M. Haldane
Princeton University, NJ, USA

J. Michael Kosterlitz
Brown University, Providence, RI, USA

“for theoretical discoveries of topological phase transitions and topological phases of matter”

They revealed the secrets of exotic matter
Quantized Hall Conductance in a Two-Dimensional Periodic Potential

D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs
Department of Physics, University of Washington, Seattle, Washington 98195
(Received 30 April 1982)

The Hall conductance of a two-dimensional electron gas has been studied in a uniform magnetic field and a periodic substrate potential \( U \). The Kubo formula is written in a form that makes apparent the quantization when the Fermi energy lies in a gap. Explicit expressions have been obtained for the Hall conductance for both large and small \( U/\hbar \).

Because of the relation between the velocity operator and the derivatives of \( \hat{H} \), the Kubo formula can be written as

\[
\sigma_H = \frac{ie^2}{A \hbar} \sum_{\epsilon_{\alpha} < E_F} \sum_{\epsilon_{\beta} > E_F} \frac{(\partial \hat{H}/\partial k_1)_{\alpha\beta} (\partial \hat{H}/\partial k_2)_{\beta\alpha} - (\partial \hat{H}/\partial k_2)_{\alpha\beta} (\partial \hat{H}/\partial k_1)_{\beta\alpha}}{(\epsilon_{\alpha} - \epsilon_{\beta})^2},
\]

where \( A \) is the area of the system and \( \epsilon_{\alpha}, \epsilon_{\beta} \) are eigenvalues of the Hamiltonian. This can be related to the partial derivatives of the wave functions \( u \), and gives

\[
\sigma_H = \frac{ie^2}{2\pi \hbar} \sum \int d^2k_1 \int d^2r \left( \frac{\partial u^*}{\partial k_1} \frac{\partial u}{\partial k_2} - \frac{\partial u^*}{\partial k_2} \frac{\partial u}{\partial k_1} \right)
= \frac{ie^2}{4\pi \hbar} \sum \oint dk_j \int d^2r \left( u^* \frac{\partial u}{\partial k_j} - \frac{\partial u^*}{\partial k_j} u \right),
\]

where the sum is over the occupied electron subbands and the integrations are over the unit cells in \( r \) and \( k \) space. The integral over the \( k \)-space unit cell has been converted to an integral around the unit cell by Stokes’s theorem. For nonoverlapping subbands \( \psi \) is a single-valued analytic function everywhere in the unit cell, which can only change by an \( \pi \)-independent phase factor \( \theta \) when \( k_1 \) is changed by \( 2\pi/qa \) or \( k_2 \) by \( 2\pi/b \). The integrand reduces to \( \partial \theta/\partial k_j \). The integral is \( 2i \) times the change in phase around the unit cell and must be an integer multiple of \( 4\pi i \).

The problem of evaluating this quantum number remains. We have considered the potential

\[
U(x, y) = U_1 \cos(2\pi x/a) + U_2 \cos(2\pi y/b),
\]

both in the limit of a weak periodic potential \( |U| \ll \hbar \omega_c \) and in the tight-binding limit of a strong periodic potential. In the weak-potential limit the wave function can be written as a superposition of the nearly degenerate Landau functions in
Haldane Model

Model for a Quantum Hall Effect without Landau Levels:
Condensed-Matter Realization of the “Parity Anomaly”

F. D. M. Haldane

Department of Physics, University of California, San Diego, La Jolla, California 92093
(Received 16 September 1987)

A two-dimensional condensed-matter lattice model is presented which exhibits a nonzero quantization of the Hall conductance $\sigma^{xy}$ in the absence of an external magnetic field. Massless fermions without spectral doubling occur at critical values of the model parameters, and exhibit the so-called “parity anomaly” of (2+1)-dimensional field theories.

PACS numbers: 05.30.Fk, 11.30.Rd

\begin{equation}
H(k) = 2t_2 \cos \phi \left( \sum_i \cos(k \cdot b_i) \right) I + t_1 \left[ \sum_i \left[ \cos(k \cdot a_i) \sigma^1 + \sin(k \cdot a_i) \sigma^2 \right] \right] + \left[ M - 2t_2 \sin \phi \left( \sum_i \sin(k \cdot b_i) \right) \right] \sigma^3,
\end{equation}
Outline

• Band topology theory
  Topological insulator (TI) and
  Topological Semimetal (TS): the topological metal in 3D

TS family

• Dirac semi-metal (DSM)
• Weyl semi-metal (WSM)
• Node-line semi-metal (NLSM)
• Triply-degenerate Nodal Point semi-metal (TDNP)

Review papers on topological quantum states from first-principles calculations
Insulator & Metal from Band Theory

Cell-periodic Hamiltonian

\[ \hat{H}(\vec{k}) = e^{-i\vec{k} \cdot \vec{r}} \hat{H} e^{i\vec{k} \cdot \vec{r}} \]

\[ u_{n,\vec{k}}(\vec{r}) = e^{-i\vec{k} \cdot \vec{r}} \psi_{n,\vec{k}}(\vec{r}) \]

\[ \hat{H}(\vec{k}) |u_{n,\vec{k}}(\vec{r})\rangle = E_n(\vec{k}) |u_{n,\vec{k}}(\vec{r})\rangle \]

What are hidden/ignored?

Quantum geometrical phase revealed by M.V. Berry.
Introduction to Berry Phase

Wilson loop method

Meaning of the phase: the center of the Wannier function for 1D band insulator or the charge center

\[ \langle u_{\vec{k}_1} | u_{\vec{k}_2} \rangle \langle u_{\vec{k}_2} | u_{\vec{k}_3} \rangle \cdots \langle u_{\vec{k}_{N-1}} | u_{\vec{k}_N} \rangle \langle u_{\vec{k}_N} | u_{\vec{k}_1} \rangle = A e^{i\theta(\vec{k}_y)} \]

Berry connection

Berry Phase & Band Topology

$\theta_n(k_y)$ is the center position of the $n$'th Wannier function.

time-reversal symmetry makes $\theta(k_y)$ is doubly degenerate at $k_y=0$ and $k_y=\pi$
Magnetic Monopole & Band topology

\[ \psi_{nk}(r) = e^{i \vec{k} \cdot \vec{r}} u_{nk}(r) e^{i \phi_n(\vec{k})} \]

\[ \phi_n = \oint_C \vec{A}(\vec{k}) d\vec{k} = \iint_{S(c)} \Omega_z(\vec{k}) d\vec{k}^2 \]

\[ \vec{A}(\vec{k}) = \sum_n < nk | \vec{\nabla}_k | nk > \]

\[ \vec{\Omega}(\vec{k}) = \vec{\nabla}_k \times \vec{A}(\vec{k}) \]
Magnetic Monopole & Band topology

Insulator vs. Metal

Gauss' theorem

The adiabatic loop does not necessarily passing through the magnetic monopole.

\[
\frac{1}{2\pi} \oint_{FS} \vec{\Omega}(k) \cdot dS(k) = C_{FS}
\]

Defined on 2D Fermi surface of a 3D metallic system

Normal metal

Topological metal

Generalized from whole Brillouin zone in *insulators* to any closed manifold in crystal momentum space.


State of matter from Band Topology

**Insulator:**
- No Fermi surface

?Metal?
- Three types of Fermi surface

- **Insulators**
  - No Fermi surface
  - Normal Insulator + Topologically nontrivial Insulator

- **Metals**
  - Fermi surface
  - Normal Metal + Topological Semi-metal

- **Semi-metal (Dirac, Weyl)**
  - Fermi points (in bulk)
  - Fermi arcs (on surface)
  - Standard Model + gravity
  - Weyl Semimetal
  - Dirac Semimetal
  - Node-line Semimetal

Extended the concept of topology to metal.
Recent Research Interests

1. **Explore** new Topological Quantum States
   - **Dirac Semimetal:** \( \text{Na}_3\text{Bi (PRB’12, Science’14)} \) \( \text{Cd}_3\text{As}_2 \) (PRB’13, Nat.Mater.’14)
   - **Weyl Semimetal:** \( \text{HgCr}_2\text{Se}_4 \) (PRL’11), \( \text{TaAs} \) (3xPRX’15, Nat. Phys.’15, PRL’15, Nat. Commun.’16)
   - **Node-line Semimetal:** 3D carbon crystal (PRB’15, PRL’16), \( \text{Cu}_3\text{PdN} \) (PRL’15)
   - **Triply-Degenerated-Nodal-Point semimetal:** \( \text{TaN (PRB’16), ZrTe (PRB’16)} \)

2. **Understand** new Topological Quantum Phenomena
   - **Correlated Topological Insulator**
     - \( \text{SmB}_6 \) (PRL’12, Nat. Commun.’14)
     - \( \text{YbB}_6 \) & \( \text{YbB}_{12} \) (PRL’14)

3. **Predict** new Topological Materials
   - \( \text{Ag}_2\text{Te (PRL’11)} \)
   - \( \text{ZrTe}_5\&\text{HfTe}_5 \) (PRX’14, PRX’16), \( \text{MXene (PRB’15), ZrSiO (PRB’15)} \)
   - \( \text{TIN (PRB’14)} \)

Highly Efficient computational tools is the basis

1. Local orbital base and pseudo-potential methods
2. Wannier function analysis
3. LDA++ methods: +Gutzwiller, +DMFT etc.
4. Material database
Methodology

1. Local orbital base and pseudo-potential methods

Advantage:
+ Quickly obtain electronic structure
+ from $O(N^3)$ to $O(N)$
+ spin-orbit coupling
+ structural optimization & molecular dynamic
+ non-collinear magnetism
+ structural code & easy to be extended

Disadvantage:
+ cut-off appro. & basis completeness
+ pseudo-potential

http://www.openmx-square.org
Methodology

2. Wannier function analysis

Advantage:
+ Intuitive picture;
+ accurate minimal basis;
+ highly efficient integration

Features of our code:
+ flexible projector;
+ symmetrized


Recent developments:
1. Boundary state calculation: slab model & Green’s function method
2. Spin texture
3. Wilson loop calculation
4. Parity calculation
5. Anomalous Hall Conductivity calculation
Dirac & Weyl Fermion

**Dirac Fermion (1928) 4x4**

\[
\begin{pmatrix}
\hat{E} - c\sigma \cdot \hat{p} & 0 \\
0 & \hat{E} + c\sigma \cdot \hat{p}
\end{pmatrix} \psi = mc^2 \begin{pmatrix}
0 & I_2 \\
I_2 & 0
\end{pmatrix} \psi
\]

\[E(k) = \pm \sqrt{k^2 + m^2}\]

**Massless Dirac Fermion (1929)**

\[
H(\vec{k}) = \vec{k} \cdot \vec{\sigma} = \begin{bmatrix}
k_z & k_x - ik_y \\
k_x + ik_y & -k_z
\end{bmatrix}
\]

**Weyl fermion 2x2**

\[
E(k) = \pm \sqrt{k^2 + m^2}
\]

**Massive Dirac Fermion**

**Massless Dirac Fermion:** two Weyl Fermions with opposite topological charges “kiss”.

Dirac & Weyl Semimetal

Transition state between TI and NI in 3D

Fragile and hard to control.

3D metal with low energy exaction behaving the same as massless Dirac/Weyl fermion.

S. Murakami et al. arXiv:1006.1188
Physica E 43, 748–754 (2011)
Dirac Semimetal with Band Inversion

as “singularity point” of various topological states

“3d graphene”

Na$_3$Bi & Cd$_3$As$_2$

The only two DSMs widely studied experimentally.

4-fold

mass term

Normal OR Topological Insulator

Noncentrosymmetric & nonmagnetic Weyl Semimetal

TaAs-family (PRX’15)

2-fold

Magnetic Weyl Semimetal

A$_2$Ir$_2$O$_7$ (X. Wan et al PRB’11), HgCr$_2$Se$_4$ (PRL’11)
Fermi arcs of WSM

Fermi arcs on the surface

$Y_2Ir_2O_7$

Crystal structure of TaAs family

Both Ta and As are at 4a Wyckoff position. (0,0,u) and $u_{Ta}=0.0$.

<table>
<thead>
<tr>
<th></th>
<th>a=b</th>
<th>c</th>
<th>u</th>
</tr>
</thead>
<tbody>
<tr>
<td>TaAs</td>
<td>3.4348</td>
<td>11.641</td>
<td>0.417</td>
</tr>
<tr>
<td>TaP</td>
<td>3.3184</td>
<td>11.363</td>
<td>0.416</td>
</tr>
<tr>
<td>NbAs</td>
<td>3.4517</td>
<td>11.680</td>
<td>0.416</td>
</tr>
<tr>
<td>NbP</td>
<td>3.33242</td>
<td>11.37059</td>
<td>0.417</td>
</tr>
</tbody>
</table>

S. Furuseth, K. Selte and A. Kjekshus,
Acta Chem. Scand. 19, 95 (1965)

Hongming Weng*, Chen Fang, Zhong Fang, A. Bernevig, Xi Dai,
http://arxiv.org/abs/1501.00060 posted on Dec. 31, 2014 and

a similar work from Princeton group
http://arxiv.org/abs/1501.00755 posted on Jan. 5, 2015 and
Known properties of TaAs family

---

**NbAs**

![Graph showing the magnetic susceptibility of NbAs, NbAs₂, Nb₃Sb₂, and NbSb₂ as a function of temperature.](image)


**TaAs**

![Graph showing the magnetic susceptibility of TaPs and TaAs as a function of temperature.](image)


---

**Table V. Magnetic susceptibilities of NbP and TaP.**

<table>
<thead>
<tr>
<th>Compound</th>
<th>$T$ (°K)</th>
<th>$X_e$ ($10^{-6}$ cgs/g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>NbP</td>
<td></td>
<td></td>
</tr>
<tr>
<td>78</td>
<td>$-0.45 \pm 0.03$</td>
<td></td>
</tr>
<tr>
<td>201</td>
<td>$-0.57 \pm 0.03$</td>
<td></td>
</tr>
<tr>
<td>297</td>
<td>$-0.52 \pm 0.02$</td>
<td></td>
</tr>
<tr>
<td>373</td>
<td>$-0.55 \pm 0.03$</td>
<td></td>
</tr>
<tr>
<td>TaP</td>
<td></td>
<td></td>
</tr>
<tr>
<td>78</td>
<td>$-0.70 \pm 0.03$</td>
<td></td>
</tr>
<tr>
<td>201</td>
<td>$-0.65 \pm 0.03$</td>
<td></td>
</tr>
<tr>
<td>297</td>
<td>$-0.62 \pm 0.02$</td>
<td></td>
</tr>
<tr>
<td>373</td>
<td>$-0.59 \pm 0.02$</td>
<td></td>
</tr>
</tbody>
</table>

Band structure of TaAs

without SOC

Topological Node-Line
Semimetal
http://arxiv.org/abs/1411.2175
Surface Fermi arcs
Experimental verification
up to early of Apr. 2015 from arXiv.

2. 2015arXiv:1502.03807 Experimental realization of a topological Weyl semimetal phase with Fermi arc surface states in TaAs @Science on Jul. 16, 2015 from Princeton & Peking University
4. 2015arXiv:1502.04684 Discovery of Weyl semimetal TaAs @PRX on Jul. 16 from IOP, CAS
5. 2015arXiv:1503.01304 Observation of the chiral anomaly induced negative magneto–resistance in 3D Weyl semi–metal TaAs @PRX on Jul. 20 from IOP, CAS
7. 2015arXiv:1503.07571 Magnetotransport of single crystalline NbAs
8. 2015arXiv:1503.09188 Observation of Weyl nodes in TaAs @Nat. Phys. on Aug. 17 from IOP, CAS
9. 2015arXiv:1504.01350 Discovery of Weyl semimetal NbAs @Nat. Phys. on Aug. 17 from Princeton & Peking University
Four hallmarks of Weyl semimetal observed in TaAs

1. “Chiral anomaly”— negative magnetoresistance
   - \textbf{arXiv:1503.01304} Observation of the chiral anomaly induced negative magneto-resistance in 3D Weyl semi-metal TaAs
   - \textbf{arXiv:1503.02630} Observation of the Adler-Bell-Jackiw chiral anomaly in a Weyl semimetal

2. Fermi arcs
   - \textbf{arXiv:1502.03807} Experimental realization of a topological Weyl semimetal phase with Fermi arc surface states in TaAs
   - \textbf{arXiv:1502.04684} \textit{Discovery of Weyl semimetal TaAs}

3. Bulk Weyl nodes
   - \textbf{arXiv:1502.03807} Experimental realization of a topological Weyl semimetal phase with Fermi arc surface states in TaAs
   - \textbf{arXiv:1503.09188} \textit{Observation of Weyl nodes in TaAs}

4. Spin texture of Fermi arc
   - \textbf{arXiv:1510.07256} \textit{Observation of spin texture of Fermi arc of TaAs}
Breakthrough & Highlight of 2015

Weyl fermions are spotted at long last

To Zahid Hasan of Princeton University, Marin Soljačić of MIT, and Zhong Fang and Hongming Weng of the Chinese Academy of Sciences, for their pioneering work on Weyl fermions. These massless particles were predicted by the German mathematician Hermann Weyl in 1929. Working independently, a team led by Hasan, and another led by Fang and Weng, spotted telltale evidence.
Triply Degenerate Nodal Point

A New Massless Fermion

Weng, Fang, et al., PRB 93, 241202(R) (2016)

Point group $C_{3v}$

\[
\begin{array}{c|cccccc}
G1 & A1 & 1 & 1 & 1 & 1 & 1 & 1 \\
G2 & A2 & 1 & -1 & 1 & 1 & -1 & -1 \\
G3 & B1 & 1 & 1 & 1 & -1 & 1 & -1 \\
G4 & B2 & 1 & -1 & 1 & -1 & -1 & 1 \\
G5 & E1 & 2 & -2 & -1 & 1 & 0 & 0 \\
G6 & E2 & 2 & 2 & -1 & -1 & 0 & 0 \\
G7 & E1/2 & 2 & 0 & 1 & /3 & 0 & 0 \\
G8 & E5/2 & 2 & 0 & 1 & -/3 & 0 & 0 \\
G9 & E3/2 & 2 & 0 & -2 & 0 & 0 & 0 \\
\end{array}
\]

\[
\begin{array}{c|cccc}
G1 & A1 & 1 & 1 & 1 \\
G2 & A2 & 1 & 1 & -1 \\
G3 & E & 2 & -1 & 0 \\
G4 & E1/2 & 2 & 1 & 0 \\
G5 & 1E3/2 & 1 & -1 & i \\
G6 & 2E3/2 & 1 & -1 & -i \\
\end{array}
\]

Na$_3$Bi $\Gamma$-A $C_{6v}$
Triply Degenerate Nodal Point

WC-type
TaN, NbN, ZrTe etc.

No SOC

+SOC
Triply Degenerate Nodal Point

Winding number 2 for spin on the Fermi surface
Triply Degenerate Nodal Point

(100) surface
Triply Degenerate Nodal Point

B

B//c

Chiral anomaly

Helical anomaly

Protected by $C_3$
Weyl nodal points Co-exist with Triply Degenerate Nodal Points

Weyl points co-exist with Triply Degenerate Nodal Points

Weyl points co-exist with Triply Degenerate Nodal Points

@50meV

Weyl points co-exist with Triply Degenerate Nodal Points

(Color online) ZrTe (100) surface state with its band structure weighted

Weyl points co-exist with Triply Degenerate Nodal Points
Weyl points co-exist with Triply Degenerate Nodal Points

Weyl points co-exist with Triply Degenerate Nodal Points
Topological Semimetal Family

a New member

TDNP

[Diagram showing various types of semimetals and their relationships, including

- Four-fold degenerate Dirac node: Na$_3$Bi, Cd$_3$As$_2$
- Dirac Semimetal
- Mass
- ISB
- Cu$_3$PdN
- MTC
- TaAs
- Node-Line Semimetal
- Spinless two-fold degenerate Nodal Line
- MTC, Cu$_3$PdN, TaAs
- TaN, NbN or ZrTe

A new member is highlighted:

- a New member

References:

- arXiv:1604.08467
- arXiv:1605.05186

Thank you for your attention!