A Brief Survey of MURI-supported research in Ong-Cava group
Z2 Topological Insulators, Dirac Semimetals, Kagome Lattice

N. Phuan Ong, Princeton University

1. Dirac and Weyl Metals
   High mobility and giant MR in Cd3As2

2. Thermal Hall current in a ferromagnet
   Spin waves and the Berry curvature in 2D Kagome ferromagnet

3. Anomalous Hall effect in ultrathin films Cr-doped (Bi,Sb)2Te3

Tian Liang, Jun Xiong, Max Hirschberger, Minhao Liu, Ali Yazdani and N.P.O. (Physics, Princeton)
Quinn Gibson, R. J. Cava (Chemistry, Princeton)
R. Chisnell, Young Lee and Dan Nocera (MIT)
Anthony Ricardella, Nitin Samarth (Physics, Penn State U)

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Out of Z2-land

Topological ideas are migrating from Z2-TRI matter to other classes of matter. The virus is the Berry curvature (Chern flux).
Weyl Semimetal

Superficially, 3D analog of graphene, but with important differences:

- No mass term $M\sigma_z$ possible (compare Boron Nitride), so always massless
- Only way to remove nodes is by pairwise annihilation
- Requires broken TRI or broken Inversion
- Must come in pairs with $\chi = \pm 1$
- Regard as monopole source or sink of Berry curvature (Chern) flux

\[
\chi = \frac{1}{2\pi} \oint \mathbf{F}(\mathbf{k}).d\mathbf{S}(\mathbf{k})
\]

Berry curvature

\[
\mathbf{F}(\mathbf{k}) = \nabla_k \times \mathbf{A}(\mathbf{k}), \quad \mathbf{A}(\mathbf{k}) = i(\mathbf{u}_k | \nabla_k \mathbf{u}_k)
\]

Wan, Turner, Vishwanath, PRB 2011
In $\text{Cd}_3\text{As}_2$, we have 4 stacks of small cubes with helical vacancy order, 2 left-handed and 2 right-handed.

Inversion symmetry *broken*
Ultrahigh mobility in Dirac semimetal Cd$_3$As$_2$

Harvested crystals come in 2 sets, A and B

- Set A --- 50 $\mu$Ωcm at 4 K
- Set B --- 30 nΩcm at 4 K

Mobility $\mu$

- 15,000 to 26,000 cm$^2$/Vs in A
- $10^6$ cm$^2$/Vs in B

- In same league as Bi 2DEG in GaAs
Giant MR extends above room temp

At all $T \to 300$ K, MR is much larger than $T$ dependence.
Giant H-linear MR is suppressed when $\mathbf{H}$ is parallel to $\mathbf{E}$.

$R_{xx}$ increases by 50-100 (H=0 to 10 T)
1. Large H-linear positive MR $H$ has component perp to $c$
   Scales like
   \[ \sigma(H, \theta) = \sigma(H \sin \theta, 90^\circ) \quad |\theta| > 20^\circ \]
   However, Zeeman energy also contributes to MR
   In weak $H$, Zeeman energy term dominates (MR is isotropic)

2. Charge pumping between Weyl nodes predicted to give negative MR

   \[ \dot{Q} = - \frac{L^2}{2\pi \ell_B^2} \frac{L e \dot{k}}{2\pi} = -V \frac{e^3}{4\pi^2 \hbar^2} E \cdot B \]

   Masked by much larger transverse positive MR. Need higher $H$?
Charge pumping and the chiral anomaly

\[ E_n = v_F sgn(n) \sqrt{2 \hbar |n| eB + (\hbar k \cdot \hat{z})^2}, \quad n \neq 0 \]

\[ E_0 = -\chi \hbar v_F k \cdot \hat{z}, \quad n = 0 \]

Charge is pumped from left to right-handed Weyl node at the rate

\[ \dot{Q} = -\frac{L^2}{2\pi \ell_B^2} \frac{Le\dot{k}}{2\pi} = -V \frac{e^3}{4\pi^2 \hbar^2} E \cdot B \]

Chiral (Adler-Bell-Jackiv) anomaly

\[ \partial_\mu j_\mu^\chi = -\chi \frac{e^3}{32\pi^2 \hbar^2} \epsilon^{\mu\nu\rho\lambda} F_{\mu\nu} F_{\rho\lambda} \]

Decay of neutral pi-meson \( \pi^0 \rightarrow 2 \gamma \), non-conservation of axial current

Why are all neutrinos left-handed?

Goldstone mode of quark condensate

Topological origin
Evidence for charge pumping and chiral anomaly?

When $\mathbf{E} \parallel \mathbf{H}$, chiral anomaly term is a maximum. Appears to cancel nearly all of the giant H-linear transverse MR. May dominate at larger H.
Back scattering by impurities suppressed at $H = 0$

Giant $B$-linear MR observed with $\mathbf{E}$ perp. to $\mathbf{B}$ (100-fold in 15 T)

Nearly $T$-independent except in weak $B$

Impurity scattering dominates phonons at finite $B$

Protection against impurity scattering at $B = 0$

Why is mobility so high in a unit cell with 80 atoms?
Theory of the Thermal Hall Effect in Quantum Magnets

Hosho Katsura,¹ Naoto Nagaosa,¹,² and Patrick A. Lee³

Hall effect of neutral currents from Berry curvature

\[ H_{\text{ring}} = -\frac{24 t^3}{U^2} \sin \Phi \vec{S}_i \cdot (\vec{S}_j \times \vec{S}_k), \]

Chirality \( \chi = S_1 \cdot S_2 \times S_3 \)

\[ \delta^2 \chi = \langle S_i \rangle \cdot \delta S_j \times \delta S_k + \langle S_j \rangle \cdot \delta S_k \times \delta S_i + \langle S_k \rangle \cdot \delta S_i \times \delta S_j \]

2nd order Fluctuations of chirality give Hall effect except they cancel exactly in all “dense” lattices

“No-Go” theorem

For triangular and square lattices, each bond contributes with opposite signs to each plaquette, so mutually cancel.

For Kagome and pyrochlore lattices, cancellations do not occur.
\[ h_\Delta = -J(S_i \cdot S_j + S_j \cdot S_k + S_k \cdot S_i) - \frac{K}{S} S_i \cdot S_j \times S_k \]
\[ \tan(\phi/3) = K/J \]

Holstein-Primakoff transform \( S_i \) to boson operators \( b_i \)

Berry curvature gives bosons an anomalous velocity, which gives Hall effect

Estimated thermal Hall conductivity

\[ \kappa_{xy} = \frac{\pi \phi}{36\sqrt{3}} T \]

Analogous to anomalous Hall effect (\( H \) merely to align \( M \) domains)

Kxy first observed by Onose, Tokura, et al.
In pyrochlore (Science 2010)
Cu(1,3-benzenedicarboxylate)

In-plane exchange: -O-C-O-

Interplane exchange:
-O-C-C-C-C-C-O-

frustrated, but orders ferromagnetically at 1.8 K
The thermal conductivity $\kappa_{xx}$ of Kagome ferromagnet Cu(1,3-bcd)

Large spin-wave current (6% of max phonon current) observed below 10 K.

Rather $H$ dependent (next slide).
H dependence of $\kappa_{xx}$ and $\kappa_{xy}$

Max Hall angle $\kappa_{xy}/\kappa_{xx} \sim 8\%$

Strong fluctuations in both $\kappa_{xx}$ and $\kappa_{xy}$ above $T_c = 1.8$ K
Observe transition from H-linear Hall signal (paramagnetic) to spontaneous signal (ferromagnetic)
Thermal analog of the Anomalous Hall Effect

Thermal Hall signal $W_{xy}$ is analog of Hall resistivity $\rho_{xy}$

Signal changes sign at $H = 0$ with magnetization

T = 1 K

Ferromagnetic magnon branch suppressed above 5 T at 1 K.
Note persistence of small Hall signal above 5 T!
\[ \sigma_{xx} \left( \frac{e^2}{h} \right) \]

vs.

\[ \mu_0 H (T) \]
The graph depicts the relationship between $V_g$ (V) and $\sigma_{xx, \min}$ (e$^2$/h) for classical, raw, and interpolated data, showing how these quantities vary with applied gate voltage.
3D Dirac semimetal Cd$_3$As$_2$
Ultrahigh mobility $\mu > 10^6$ cm$^2$/Vs (Set B). Carriers protected from back scattering in zero magnetic field

In Kagome ferromagnet Cu(1,3-bcd), see a large thermal Hall conductivity. Hall angle (max) $\sim$ 8%. Consistent with predictions of Katsura, Nagaosa and Lee.

Considerable progress in observing anomalous Hall effect in ultrathin (Bi,Sb)$_2$Te$_3$ doped with Cr grown on STO. Tunable across Dirac point by backgate.
END
Sample A2

\( \mu_0 H (T) \)

\( \rho_{xx} \) (m\( \Omega \) cm)

\( \sigma_{xx} \) (10\(^3\) \( \Omega^{-1} \) cm\(^{-1} \))

\( \theta = 0^\circ \)

\( \theta = 5^\circ \)

\( H^1 \)
Three Dimensional Dirac Semimetal and Quantum Spin Hall Effect in Cd$_3$As$_2$

Zhijun Wang, Hongming Weng,* Quansheng Wu, Xi Dai, and Zhong Fang†

IOP, Beijing

4x4 basis set

$|S,\frac{3}{2}\rangle, |P,\frac{3}{2}\rangle, |S,-\frac{3}{2}\rangle, |P,-\frac{3}{2}\rangle$

$$H_\Gamma(k) = \epsilon_0(k) + \begin{pmatrix}
M(k) & Ak_+ & 0 & B^*(k) \\
Ak_- & -M(k) & B^*(k) & 0 \\
0 & B(k) & M(k) & -Ak_- \\
B(k) & 0 & -Ak_+ & -M(k)
\end{pmatrix}.$$
Fermi velocity derived from SdH amplitude vs temp

Dingle temp $\Rightarrow$ cyclotron mass $m_c$. For Dirac dispersion $m_c = E/v^2$
Crystals in Set A

Resistivity \( \sim 50 \, \mu\Omega \text{cm} \) at 4 K
RRR \( \sim 5 \)
Mobility \( \mu = 15,000 \) to \( 26,000 \, \text{cm}^2/\text{Vs} \)

Hall density \( n_H \sim 2 \times 10^{18} \rightarrow 2 \times 10^{19} \, \text{cm}^{-3} \)

Only one band (?) of carriers \( (n\)-type)\)

Giant \( H \)-linear transverse MR

Expt difficulty: Large Hall voltage skews the MR curves
If TRI is restored → Weyl points of opposite chirality mutually annihilate
Left with a gapped spectrum

However, if crystalline symmetry prevents annihilation, we have a 4-comp Dirac metal

Each node is a 4-comp massless Dirac point
Has 4-fold degeneracy (lifted by breaking of TRI or Inv.)
3D Analog of graphene
Berry Curvature in Crystalline Solids

<table>
<thead>
<tr>
<th>Berry vector potential $A(k)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A(k) = (u_{nk}, r_{op} u_{nk}) = (u_{nk}, i \nabla_k u_{nk})$</td>
</tr>
<tr>
<td>$F(k) = \nabla_k \times A(k)$</td>
</tr>
</tbody>
</table>

Intracell position of wave-pkt (non-gauge invar)

Berry curvature $F(k)$ is gauge invariant.
An effective magnetic field living in $k$-space

$F(k)$ is pervasive in modern Cond. Matt. Phys.

1. Semiclassical eqns. of motion

$$\dot{\mathbf{k}} = e\mathbf{E} + ev \times \mathbf{B}$$

2. Intrinsic Anomalous Hall Effect

$$J_H = \int d^3k \int^0 f \mathbf{F}(k)$$

3. Integral quantum Hall Effect

$$\sigma_{xy} = \frac{e^2}{2\pi \hbar} \int_{BZ} dk_x dk_y F_z(k) = \frac{e^2}{h} C_1$$

4. Topological Hall effect in skyrmion systems

Chirality $\chi = S_1 \cdot S_2 \times S_3$
\(\mu\text{SR in spin-1/2 Kagome ferromagnet}\)

Marcipar, Amit Keren (Technion), Nytko, Nocera, Lee, Helton (MIT)  

**Cu(1,3-benzenedicarboxylate)**

In-plane exchange: \(-\text{O-C}\)

Interplane exchange: \(-\text{O-C-C-C-C-C-O}\)

**FIG. 6.** The fluctuation rate \(\nu\) versus temperature. Inset: \(\nu\) near 1.8 K on a log-log scale. The error bars are smaller than the symbol.

4x4 basis  $|S,\frac{1}{2}\rangle, |P,\frac{3}{2}\rangle, |S,-\frac{1}{2}\rangle, |P,-\frac{3}{2}\rangle$

B field also breaks TRI $\rightarrow$ Weyl nodes move apart, Lifshitz transition

Tests need higher B and higher mobility
Scaling fails for angle $\theta < 20^\circ$

Simple scaling

$$\sigma(H, \theta) = \sigma \left( \frac{H}{ \sin \theta}, 0 \right)$$

Good for $\theta > 20^\circ$
(dotted curves)
(purely orbital MR)

Fails for $\theta < 20^\circ$
Because Zeeman energy is important at low $H$

These 2 effects mask charge pumping channel
SdH oscillations in Bi$_2$Te$_2$Se in 45 Tesla field and in ionic liquid

**Left Panel:** SdH oscillations of topological Dirac states in BTS in 45 T field

**Right Panel:** Tuning of the SdH period by ionic liquid gating in field up to 32 T
• Surface electron feels surface E-field. In its rest, sees field $B = v \times E$
• Large $B$ (enhanced by SOI) locks spin $s \perp v$
• Rashba-like Hamiltonian

$$H = v_F \hat{n} \times \mathbf{k} \cdot \mathbf{s}$$

Helical, massless Dirac states with opposite chirality on opp. surfaces of crystal

Suppression of $2k_F$ scattering

Surface conductance

$$G_s = \left( \frac{e^2}{h} \right) k_F l$$

$$R_s \sim 400 \text{ Ohms} \quad \text{if } k_F l = 100$$
Limiting behavior as $1/B_n \to 0$

Intercept ($1/B \to 0$) at $n = -0.40 \to -0.55$

High-field SdH results support Dirac dispersion
Giant MR in sample B1

Trans. MR very large
1000-fold incr at 15 T

$R_{xx} \sim H^{2.5}$
not $H$-linear

May have a second $n$-type band

Mobility $\mu > 10^6$ cm$^2$/Vs
Quantum oscillations in high-mobility sample B1

\[ \text{Graph showing } \sigma_{xx}(Q^{-1} \text{ cm}^{-1}) \text{ vs. } \mu_0H \text{ (T)} \]

- SdH oscillations
- \( H \) perp I
- \( H^3 \)

Temperature: \( T=4.5K \)
Quantum oscillations in high-mobility sample B1

Sample B1

See spin split (or valley split) at high fields

N= 3 level is anomalously low in conductivity
\( v_F = (6 - 10) \times 10^5 \text{ cm/s} \)

\( 16 \times 10^5 \text{ cm/s} \) (Hasan)

SdH oscillations provide more accurate meas.
Sample 3

Tuning SdH oscillations by Liquid gating up to 45 Teslas

![Graph showing SdH oscillations with different gate voltages.](image)