Interplay of transport and domain walls in nodal semimetals

Leon Balents, KITP

APS March meeting, LA, 3/6/18
Collaborators

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Takehito Suzuki

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ENS Lyon
MIT
TaAs, Na$_3$Bi, TaP, WTe$_2$, ...
Why magnetic Weyls?

• Possibility to observe AHE
• Interesting correlation physics of magnetism
• Ability to affect electrons in situ by modifying magnetic configuration
• Probe static and dynamical effects of real space topological defects
Anomalous Hall Effect

Unique property of a magnetic Weyl semimetal

\[ \sigma_{xy} = \frac{e^2 k_0}{\hbar 2\pi} \]

Fermi arc = chiral edge state

obviously breaks time-reversal symmetry
need a magnetic material
Anomalous Hall Effect

Unique property of a magnetic Weyl semimetal

\[ \sigma_{\mu\nu} = \frac{e^2}{2\pi\hbar} \epsilon_{\mu\nu\lambda} Q_\lambda \]

\[ \bar{Q} = \sum_i \bar{k}_i q_i + \bar{Q}_{RLV} \]

semi-quantum AHE

obviously breaks time-reversal symmetry

need a magnetic material
Antiferromagnetic Weyls

Pyrochlore iridates

Mn$_3$Sn, Mn$_3$Ge

RAIGe

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X. Wan et al, 2011

H. Yang et al, 2017

G. Chang et al, 2016
Quasiparticles

Expect that any magnetically ordered system is described at first order by mean-field quasiparticle Hamiltonian

\[ H = H_{\text{band}} - \sum_i h_i \cdot c_i^\dagger \frac{\sigma}{2} c_i \]

effective Zeeman “exchange” field due to local ordered moment

Think of free-electron structure associated with each magnetic configuration
Mn$_3$Sn family

large ordered antiferromagnetic moment  
\[ \sim 2 \mu_B / \text{Mn} \]
tiny FM moment:  
\[ \sim 0.002 \mu_B / \text{Mn} \]

two kagomé layers of Mn, related by inversion

\[ T_N \sim 420 \text{K} \]

Nagamiya et al, 1982
Energetics: triangle

\[ E = J \left( S_1 \cdot S_2 + S_2 \cdot S_3 + S_3 \cdot S_1 \right) \]
\[ + D \hat{z} \cdot (S_1 \times S_2 + S_2 \times S_3 + S_3 \times S_1) \]
\[ - K \sum_i (\hat{n}_i \cdot S_i)^2 \]

\[ J \gg D \gg K \quad \text{Hierarchy of interactions} \]

- J: spins at 120° angles and M=0
- D: spins are “anti-chiral” in XY plane
- K: weak canting toward easy axes creates tiny moment and fixes in-plane angle
Textures

\[ \psi = |\psi| e^{i\theta} \]

\[ F \sim \int d^3 x \left\{ \frac{\rho}{2} (\nabla \theta)^2 - \lambda \cos 6\theta \right\} \]

sine-Gordon model with 6-fold anisotropy

\[ \rho \sim \frac{J}{a} \quad \lambda \sim \frac{K^3}{J^2a^3} \]
Textures

\[ \psi = |\psi| e^{i\theta} \quad F \sim \int d^3x \left\{ \frac{\rho}{2} (\nabla \theta)^2 - \lambda \cos 6\theta \right\} \]

soliton = domain wall connecting neighboring minima of cosine

\[ \theta(x) = \frac{2}{3} \tan^{-1} \exp \left( \frac{x}{\xi} \right) \quad \xi = \frac{1}{6} \sqrt{\frac{\rho}{\lambda}} \]

wide DWs
equipotentials from solution of Laplace’s equation for a Hall bar with two domains

Could use this DW as a switch??
Domain formation

quench
Domain formation

vortex

anti-vortex
Domain wall bound states

ARPES of domain wall seems challenging to say the least!

- Transport: enhanced intrinsic Hall conductivity within a DW?
- STM: signatures of bound states in LDOS?
CeAlGe

- tetragonal
- Ce $4f^1$ moments
- Semi-metallic band structure

Space group: $I4_1md$

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Takehito Suzuki
Lucile Savary
Jianpeng Liu
Band structure

- bandwidth $\sim 1$eV
- no large Fermi surface: true semi-metal
- large rare-earth d-orbital content: substantial coupling to rare earth moments
Ce moments

Ce$^{3+}$ typically Ising-like Kramers doublet

effective S=1/2 spin below
~10meV ~ 100K energy scale

4f$^1$ configuration: large orbital component and hence strong magnetic anisotropy

e.g. A. Severing et al, 1989
Magnetic order

Magnetic transition at 5K

2 Ce sublattices. Order does not enlarge unit cell
Kondo lattice scales

\[ H = H_{\text{band}} + J_K \sum_i S_i \cdot c_i^\dagger \frac{\sigma}{2} c_i \]

RKKY

\[ J_{RKKY} \sim \frac{J_K^2}{E_F} \]

\[ J_K \sim \sqrt{J_{RKKY}E_F} \quad \sim 100\text{meV} \]

5K 1eV
Summary: key features

• Semi-metal
• Small bandwidth ~ 1eV
• Large $J_K \sim 100\text{meV}$
• Strong magnetic anisotropy/SOC
• Low $T_N \sim 5\text{K}$
Magnetization

- In-plane field shows ferromagnetic component
- Out of plane field paramagnetic
- If you look carefully, hints of more transitions
Resistivity

resistivity enhancement at intermediate fields and low T
Resistivity

Very narrow angular dependence!
Suzuki Angular Magneto-Resistance
Suzuki Angular Magneto-Resistance
Savary Angular Magneto-Resistance
Suzuki Angular Magneto-Resistance
Savary Angular Magneto-Resistance
Singular Angular Magneto-Resistance

SAMR
Effect is tied to crystalline axes. Yet appears only below critical temperature.

Must be some effect of space group symmetry breaking. Unique to \(<100>\) axis?
Symmetry

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Table 2: All transformations for $\mathbf{h}$. 
Fields along <100> axes preserve this "magnetic mirror" symmetry.

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Table 2: All transformations for h.
Minimal model

Two Ce sublattices

"intra-unit cell antiferromagnet"

\[ E = J_\perp (S_A^x S_B^x + S_A^y S_B^y) + J_z S_A^z S_B^z + \sum_\alpha [D (S_\alpha^z)^2] \]
Minimal model

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\]

\[2D > J_z - J_p\] in-plane (XY) spins
Spin Flop

Standard Heisenberg or XY antiferromagnet
Minimal model

Two Ce sublattices

"intra-unit cell antiferromagnet"

\[
E = J_\perp (S_A^x S_B^x + S_A^y S_B^y) + J_z S_A^z S_B^z + \sum_\alpha \left[ D (S_\alpha^z)^2 - \mathbf{H} \cdot \mathbf{m}_\alpha \right],
\]

\[
\mathbf{m}_\alpha = g_\alpha \mathbf{S}_\alpha
\]

\[
g_A = \begin{pmatrix}
g_x \\
g_y \\
g_z
\end{pmatrix},
\]

\[
g_B = \begin{pmatrix}
g_y \\
g_x \\
g_z
\end{pmatrix}
\]
Minimal model

Two Ce sublattices

“intra-unit cell antiferromagnet”

\[
E = J_\perp (S_A^x S_B^x + S_A^y S_B^y) + J_z S_A^z S_B^z + \sum_\alpha D (S_\alpha^z)^2 - \mathbf{H} \cdot \mathbf{m}_\alpha,
\]

\[
\mathbf{H} = (H, 0, 0)
\]

\[
E = J_\perp (S_A^x S_B^x + S_A^y S_B^y) - H (g_x S_A^x + g_y S_B^x)
\]
Spin Flop

With g-factor anisotropy and $H$ along (100)
Spin Flop

$m_{010} \times TR$
broken
Domains

$m_{010} \times TR$

broken

or

$S_{x}^{y} \rightarrow -S_{x}^{y}$
Minimal model

Two Ce sublattices

"intra-unit cell antiferromagnet"

\[ E = J_\perp (S_A^x S_B^x + S_A^y S_B^y) + J_z S_A^z S_B^z + \sum_\alpha [D (S_\alpha^z)^2 - \mathbf{H} \cdot \mathbf{m}_\alpha] , \]

\[ \mathbf{m}_\alpha = g_\alpha \mathbf{S}_\alpha \]

\[
\begin{align*}
g_A &= \begin{pmatrix} g_x & g_y & g_z \end{pmatrix} \\
g_B &= \begin{pmatrix} g_y & g_x & g_z \end{pmatrix}
\end{align*}
\]
Domains

$m_{010} \times \text{TR} \hspace{1cm} \text{broken explicitly}$
Phase diagram

Canted phase forms 4 “infinitely thin” wedges
Phase diagram
Phase Diagram

\[ \mu_0 H(T) \]

\[ T(K) \]

\[ \delta \rho_{xx}(\mu \Omega \text{cm}) \]
Resistivity

Extra resistance comes from domain walls

\[ \rho_{\text{eff}} = \rho + \frac{\tilde{\rho}_{\text{dw}}}{\ell_d} \]

\[ V_{\text{dw}} = \tilde{\rho}_{\text{dw}} j \]

Size of the effect depends on size of \( \tilde{\rho}_{\text{dw}} \)
Domain wall

Strong anisotropy/Ising order:
narrow domain walls

Crudely, effective potential for electrons is “abrupt”: strong scattering if Fermi energy is low
Bound states at domain walls, while interesting, are hard to directly observe. More easily observed are effects of transport across a wall, e.g. the resistance of a domain wall. Some simple considerations, which we now detail, suggest the latter is an interesting quantity for these types of materials. Consider a flat domain wall located on the plane $x = 0$ in three dimensions. The two domains are related by one of the spontaneously broken symmetries of the system, which is a space group operation. Far from the domain wall, i.e. at $x \approx \pm 1$, the system is translationally invariant and in one of these two states. In each domain, we can define a band structure, which depends in detail on the form of the magnetic order, and is different in the two cases. The low energy physics, most importantly transport, is governed by the electronic states near the Fermi energy. These form one or more Fermi surfaces in either case. If the operation relating the two domains is other than translation, then the Fermi surfaces are different, and related by the corresponding operation on the momentum.

We apply the Landauer-Büttiker formalism for the transport across the wall, imagining a sample of cross-sectional area $L^2$ in the $y$-$z$ plane and infinite in $x$. This is effectively a multi-channel 1d conductor, with $L^2$ channels given by the quantized momenta $k^y, k^z$ for the transverse directions. Accordingly, the conductance $G_{xx}$ in the $x$-direction is equal to

$$G = \sum_{n=1}^{L^2} g_n \frac{e^2}{h},$$

where $g_n$ is the transmission of the $n$th mode of the conductor at the Fermi energy. Fermi surfaces do not span the whole Brillouin zone and so modes do not exist at the Fermi energy at all momenta. A necessary condition for any non-zero transmission is that a mode exists at the Fermi energy on both sides of the domain wall. Geometrically, this condition requires that the projections of the two Fermi surfaces onto the $k^y-k^z$ plane of the domain wall both contain the momentum of the quantized mode $k^y, k^z$. Taking into account only the non-vanishing contributions, Eq. (1) becomes

$$G = L^2 A_{\text{int}} \left(2 \pi \right)^2 \frac{e^2}{h},$$

where $A_{\text{int}}$ is the intersection area in momentum space, and $T<1$ is the average transmission of the geometrically-allowed modes. Now it is apparent that a large domain wall resistance appears when the Fermi surface overlap is small. For example, in the limit of an ideal Weyl semimetal with pointlike Fermi surfaces, if the Weyl points are in different positions in the two domains, the overlap is zero and the conductance vanishes!

The proportionality of the conductance to $L^2$ is what is expected classically for a conductor, so Eq. (2) can just be interpreted in terms of an intrinsic relation between the current density $j = I/L^2$ across the domain wall and the corresponding voltage drop, $V = G_j$, where $\tilde{\tau}_{dw} = L^2/G$ in Eq. (2).

It may be instructive to use this to estimate the contribution of domain walls to the bulk resistivity. Crudely modeling the transport through a mosaic of domains of typical size $\lambda_d$ as a 1d stack of domain walls with the usual current-voltage relation and a bulk resistivity $\tau$, we obtain

$$\tau_e \approx \tau + \tilde{\tau}_{dw} \lambda_d = \tau + \left(2 \pi \right)^2 A_{\text{int}} \frac{\tau}{\hbar e^2}.$$

Using the usual Drude estimate $\tau \approx h/e^2 k_F^2$, where $\lambda_d$ is the usual mean free path, we find that the fractional change in resistivity due to domain walls is of order

$$\tau_e \approx \tau + \left(2 \pi \right)^2 A_{\text{int}} \lambda_d \tau \frac{1}{h e^2 k_F^2}.$$
Phase space

Fermi surfaces differ by $m_{010} \times TR$
Weyl points

Low symmetry, SOC: Weyl point locations depend on domain

(from DFT-fit tight-binding model)
Phase space

Fermi surfaces differ by $m_{010} \times TR$

projection to interface BZ

Only overlapping portions contribute!
Using the usual Drude estimate to stack of domain walls with the usual current-voltage relation and a bulk resistivity when the Fermi surface overlap is small. For example, in the limit of an ideal Weyl semimetal the geometrically-allowed modes. Now it is apparent that a large domain wall resistance appears due to two Fermi surfaces onto the both sides of the domain wall. Geometrically, this condition requires that the projections of the Fermi surfaces do not span the whole Brillouin zone and so modes do not exist at the Fermi energy at all momenta.

Translation, then the Fermi surfaces are different, and related by the corresponding operation on different positions in the two domains, the momentum of the plane of the domain wall both contain the momentum of the mode of the conductor at the Fermi energy. Fermi surfaces differ by \( m_{010} \times TR \).

It may be instructive to use this to estimate the contribution of domain walls to the bulk effects of transport, is governed by the electronic states near the Fermi energy. These form and in one of these two states. In each domain, we can define a band structure, which depends in considerations, which we now detail, suggest the latter is an interesting quantity for these types of effects of transport.

\[
G = L^2 \frac{A_{int}}{(2\pi)^2} T \frac{e^2}{h}.
\]

\[
\frac{\rho_{eff} - \rho}{\rho} \sim \frac{1}{k_F A_{int} \ell_d} \ell T^{-1}
\]
Super Amazing Magneto-Resistance: a new effect in a SOC semimetal

?One of many new effects related to topological defects in semimetals?

Other talks:
- C44.00001
- K10.00001
- K10.00002