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Title: Intersections of quantum matter

Author(s): Grefe, Sarah Elaine

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Intersections of quantum matter

Sarah E. Grefe

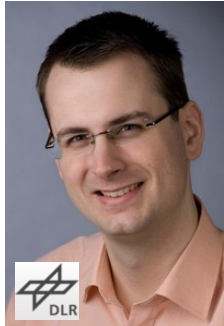
Friday February 24, 2023

LA-UR-XX-

Acknowledgements



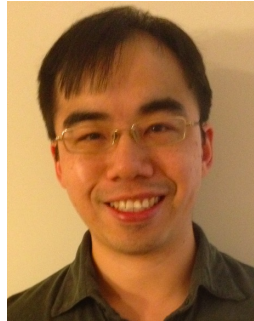
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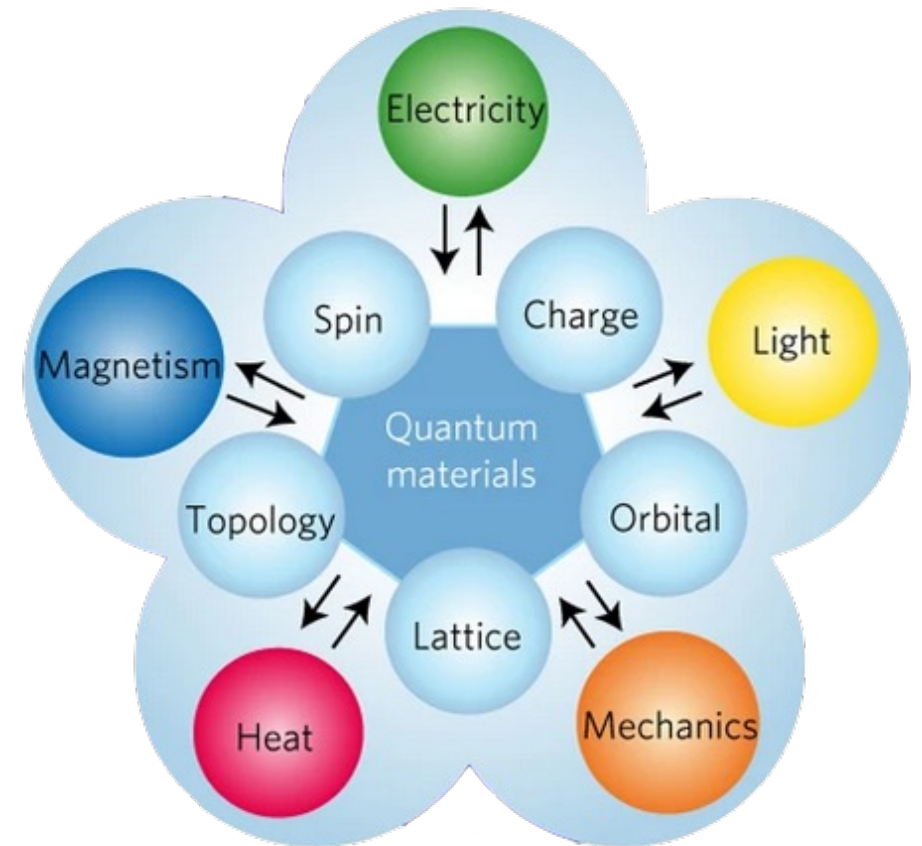


Diego Zocco



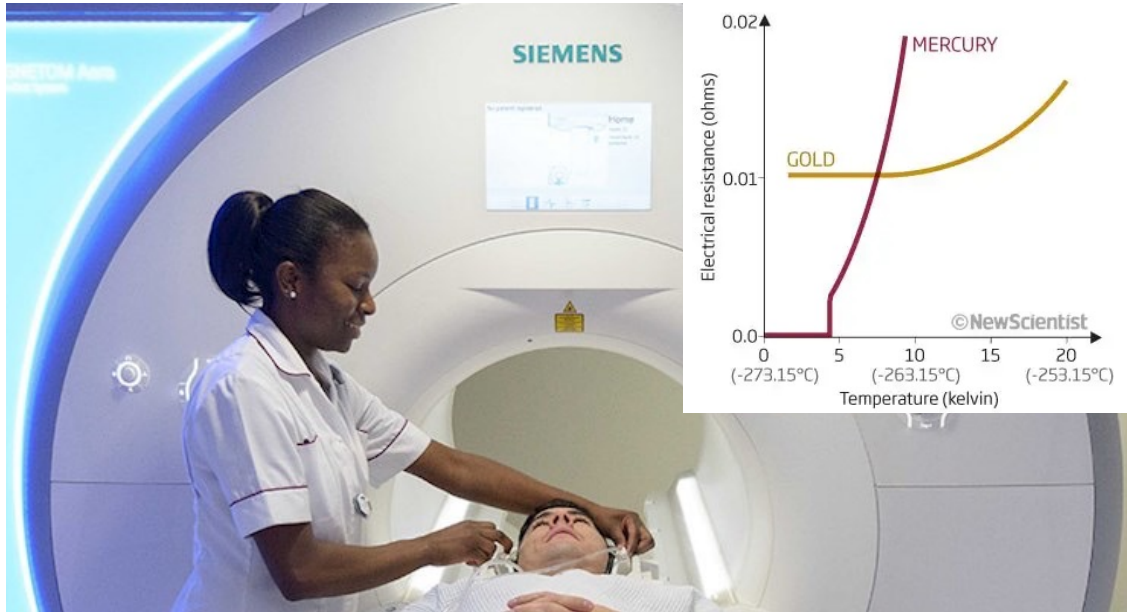
Quantum matter: asking “why?”

- Fundamental particle properties
- Collective: from many to one
- Condensed matter physics frontiers

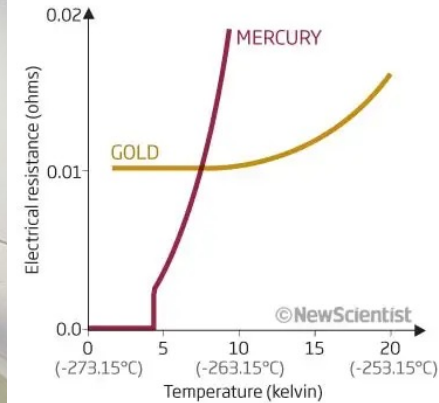


Discovery → commercial: superconductivity

Zero resistance < T_c (1911)



Magnetic Resonance Imaging (1980)



Meissner effect (1933)

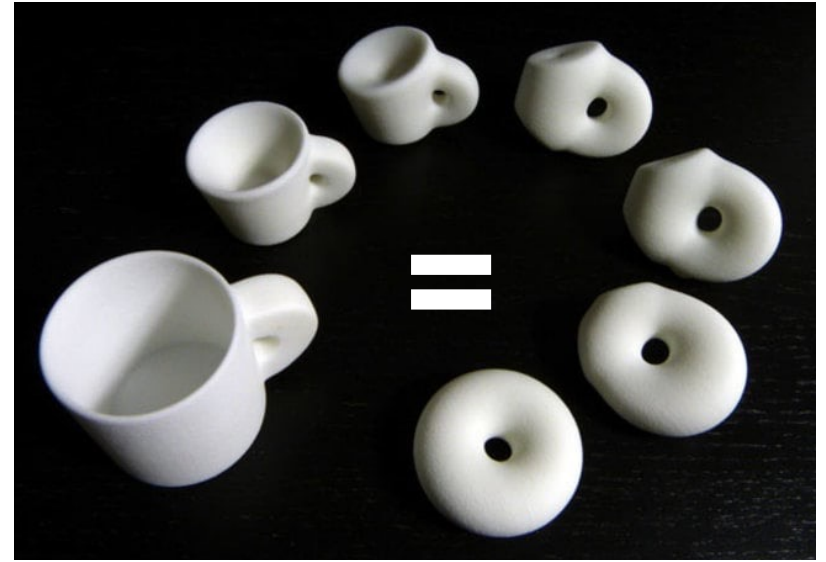
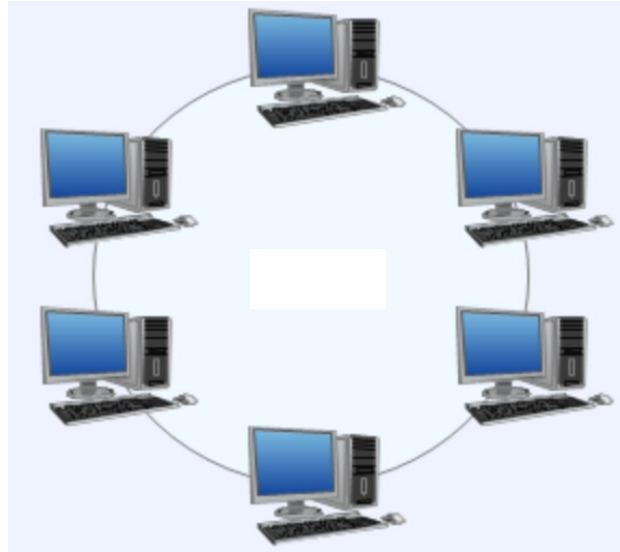


SCMagLev Trains (2027)

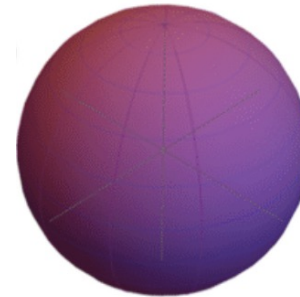
Topology



≠



≠

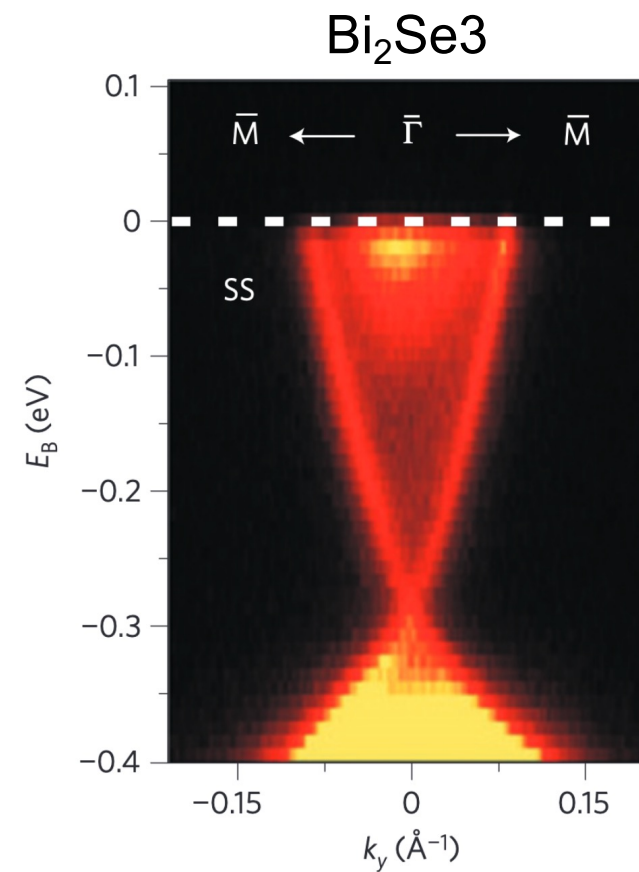
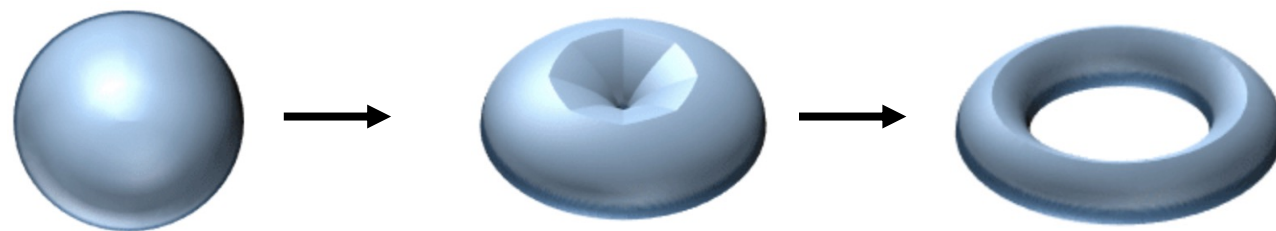
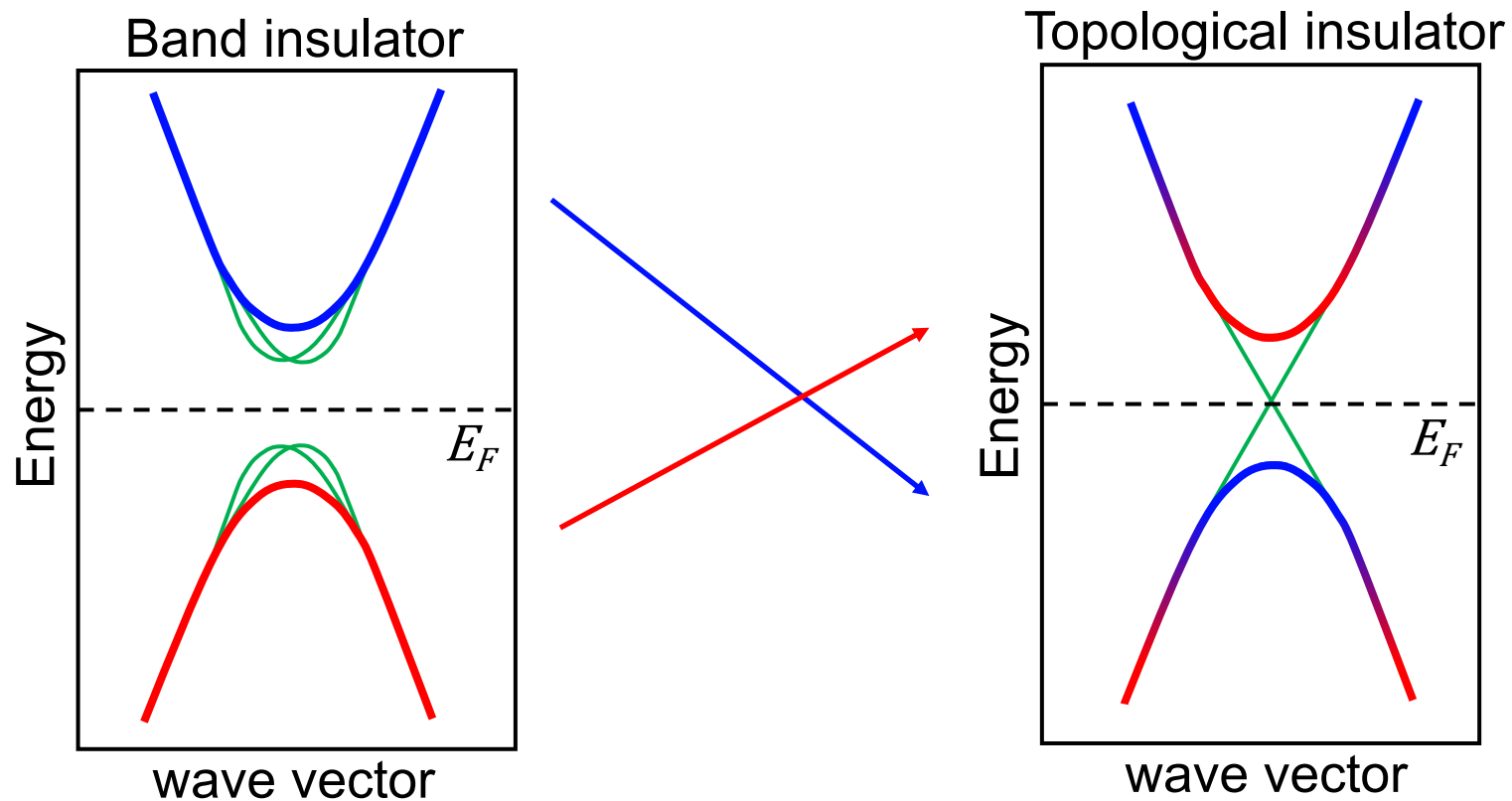


≠



≠

Topological matter



Electron interactions

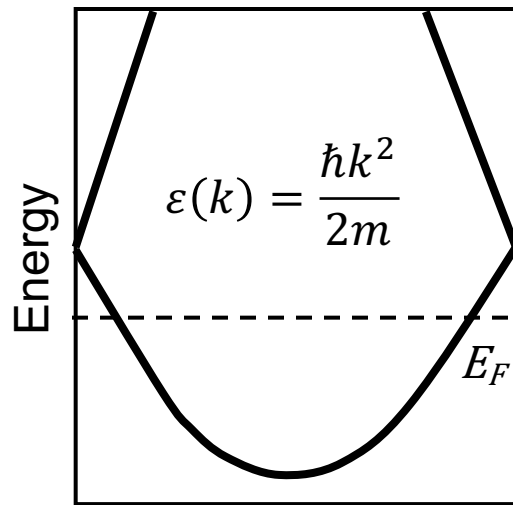
Interaction strength: U/D



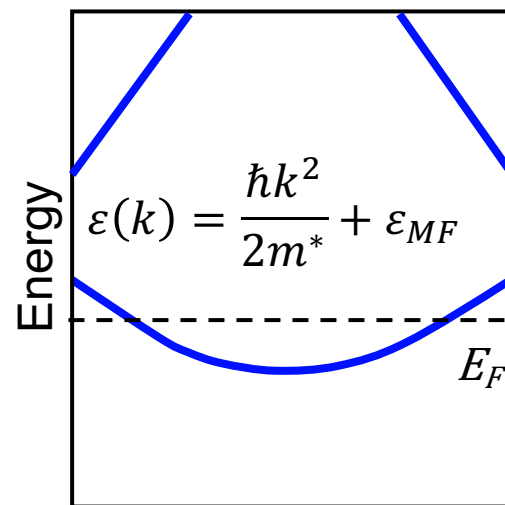
Non-interacting:
Bloch waves

Weak:
Fermi liquid

Strong:
Depends!



wave vector

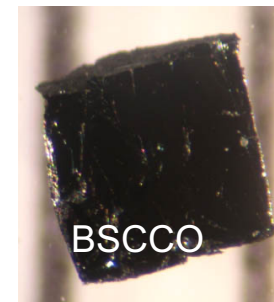


wave vector



Magnetism

$$H(\sigma) = - \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j - \mu \sum_j h_j \sigma_j$$



High- T_c
superconductivity

$H = ???$

Outline

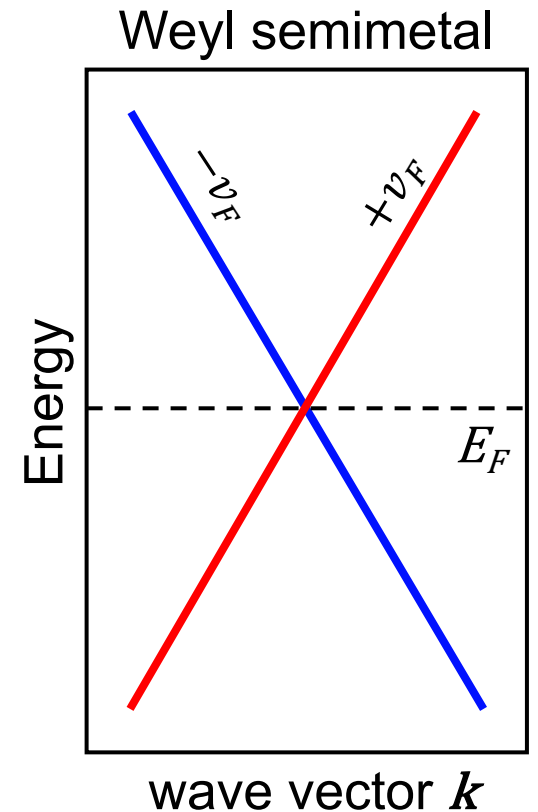
1. Topological Weyl semimetal
2. Strongly correlated Kondo physics
3. The Weyl-Kondo semimetal
4. Future projects

Hermann Weyl's equation

Dirac (1928), massive relativistic spin-1/2: $i\hbar\gamma^\mu\psi - mc\psi = 0$

Weyl (1929), massless relativistic spin-1/2: $i\hbar\frac{\partial\psi}{\partial t} = \pm c\boldsymbol{\sigma} \cdot \mathbf{p}\psi$

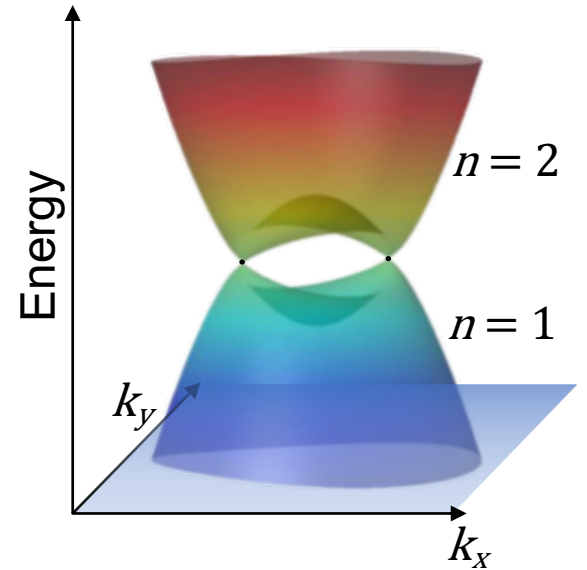
Herring (1937), crystal eigenenergy touching: $\hat{H} = \pm v_F\boldsymbol{\sigma} \cdot \mathbf{k}$



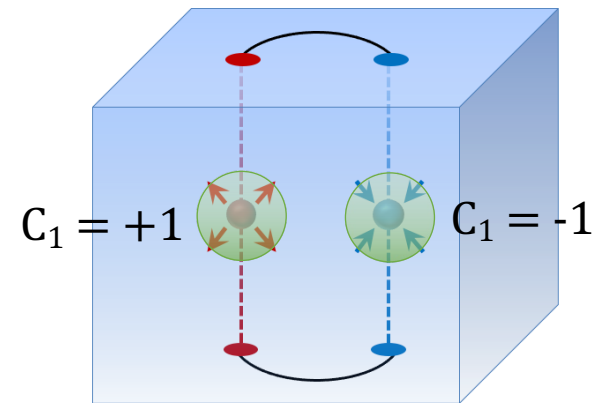
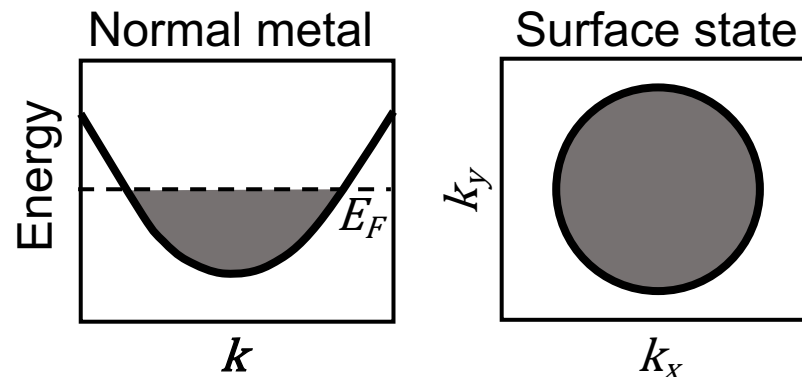
How do we know it's topological?

Topological invariant:
$$C_n = \frac{1}{2\pi} \int_{dS} \boldsymbol{\Omega}_n(\mathbf{k}) \cdot d\mathbf{S}$$

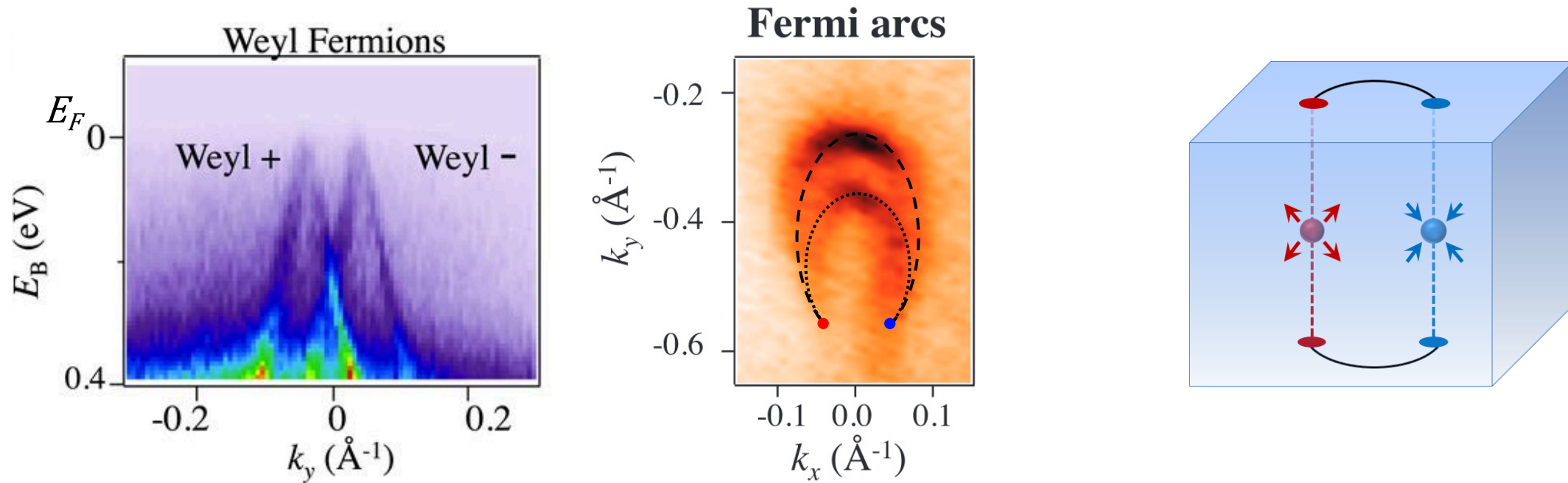
Berry curvature:
$$\boldsymbol{\Omega}_n(\mathbf{k}) = i \langle \nabla_{\mathbf{k}} u_{n\mathbf{k}} | \times | \nabla_{\mathbf{k}} u_{n\mathbf{k}} \rangle$$



Bulk-surface correspondence:



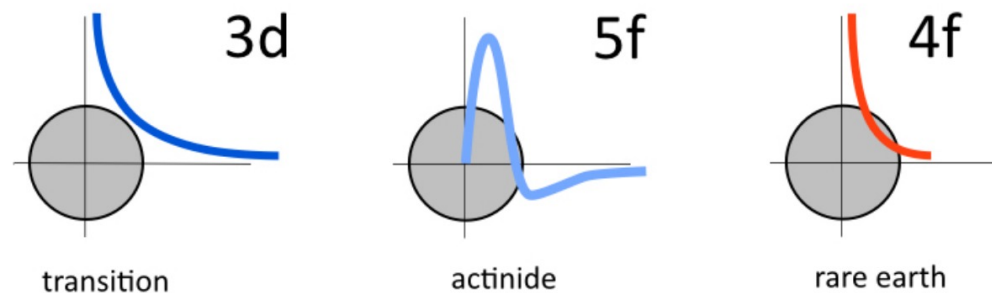
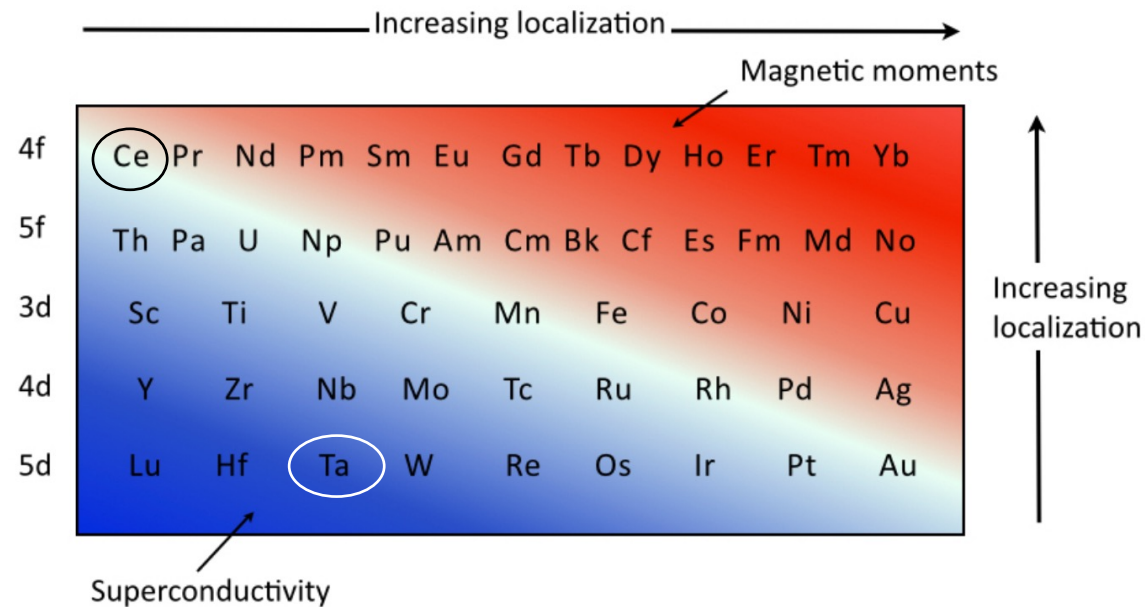
The Weyl semimetal is observed



Xu et al., Science 349:6248 (2015)

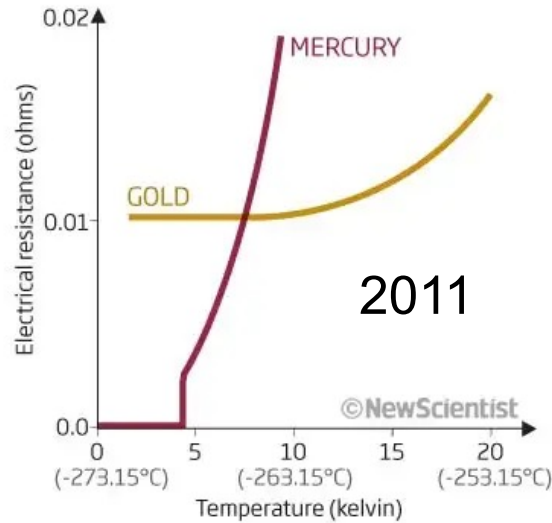
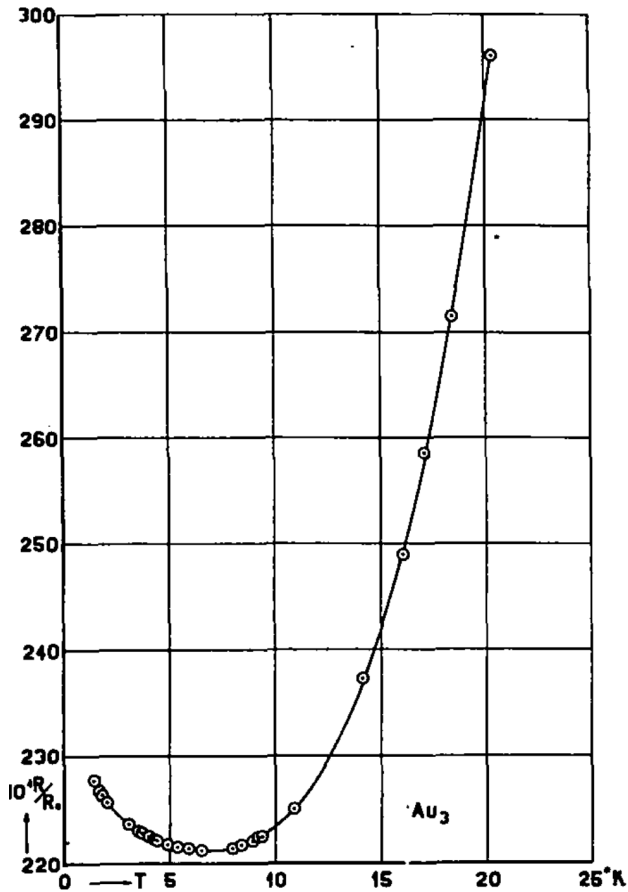
Lu et al. Science 349:6248 (2015)
Lv, et al. PRX 5:031013 (2015)

Strongly correlated matter



The Kondo effect

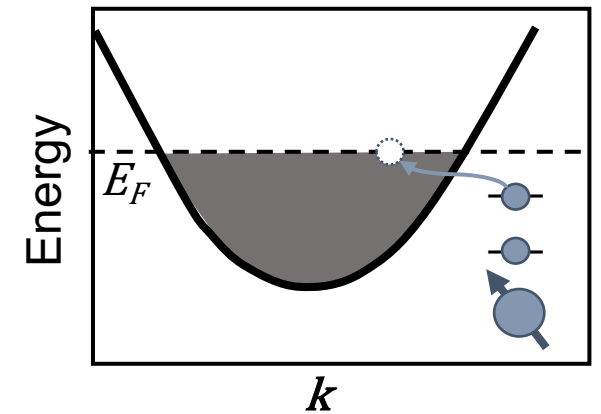
Resistance of gold vs T



1936: **Magnetic** impurities

Kondo (1964)

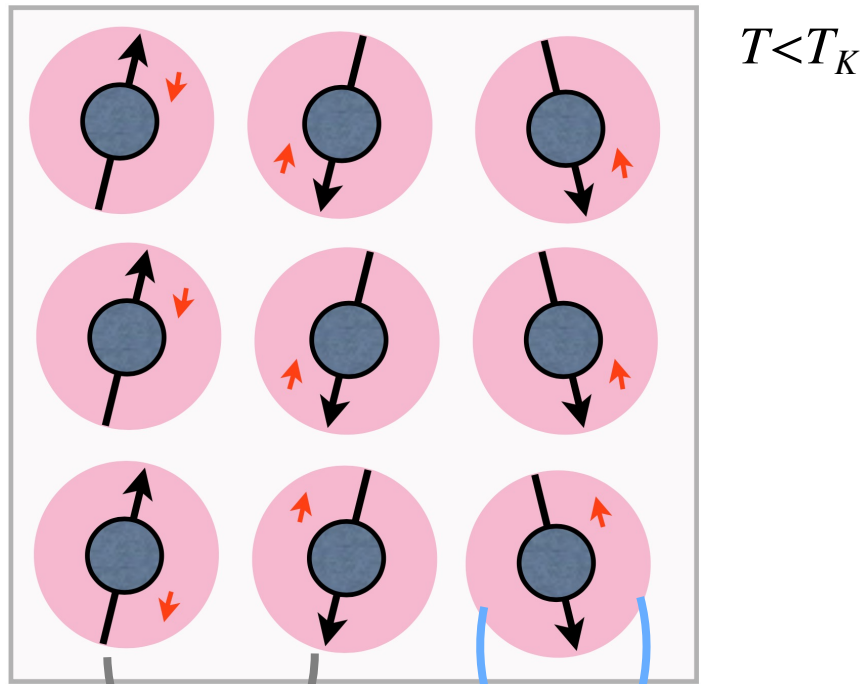
Metal + Magnetic ion



$$\rho(T) \sim \rho_{FL} + \rho_{LV} + c_m \ln \frac{\mu}{T}$$

$$T < T_K$$

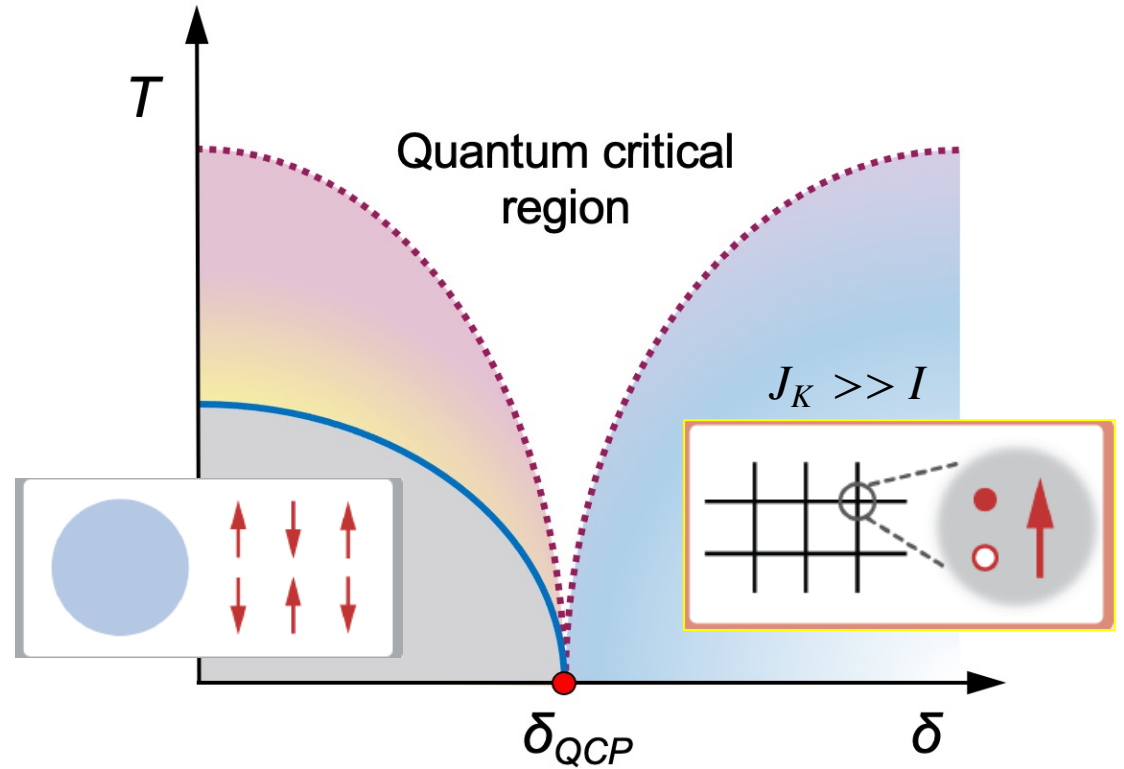
Heavy fermion systems



AFM: I

Kondo: J_K

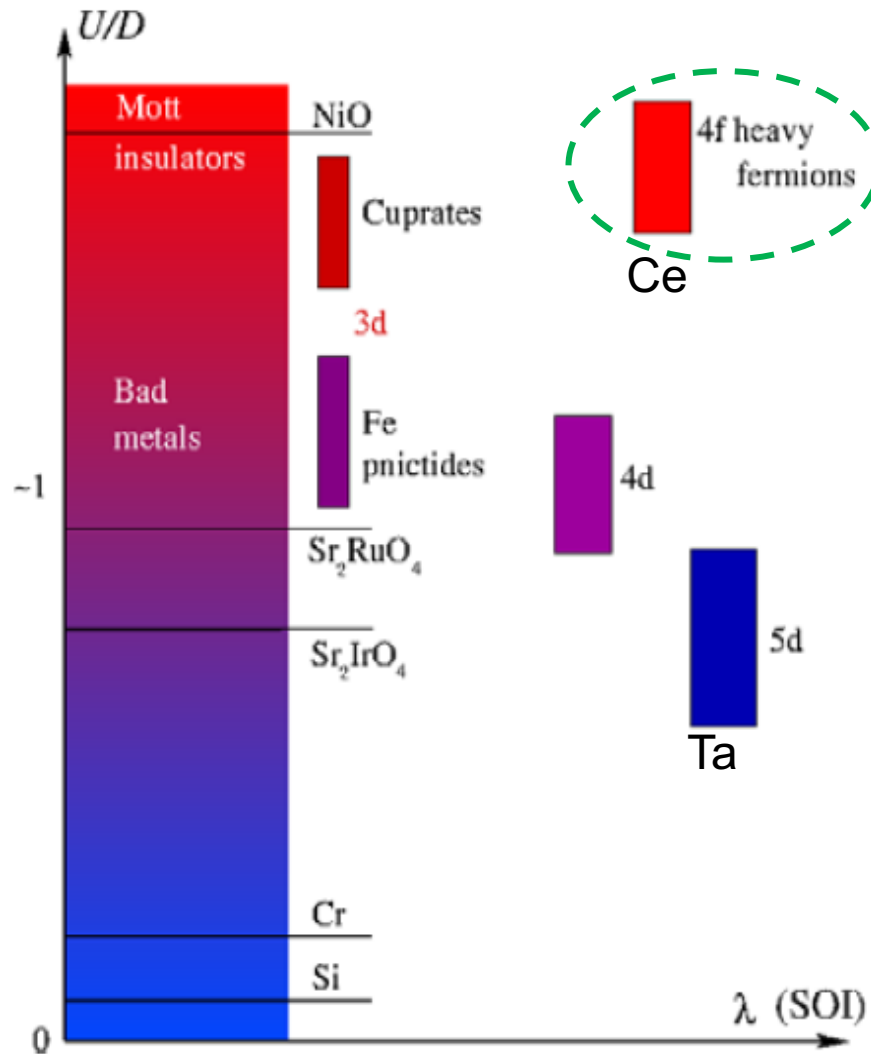
$$\delta = J_K/I$$



Why 'heavy'?

- $C \propto \gamma T$
- $\gamma \propto m^*$

Topology across the correlation spectrum



Will strong correlations
destroy topological
semimetal states?

Heavy fermion system
+
Weyl semimetal

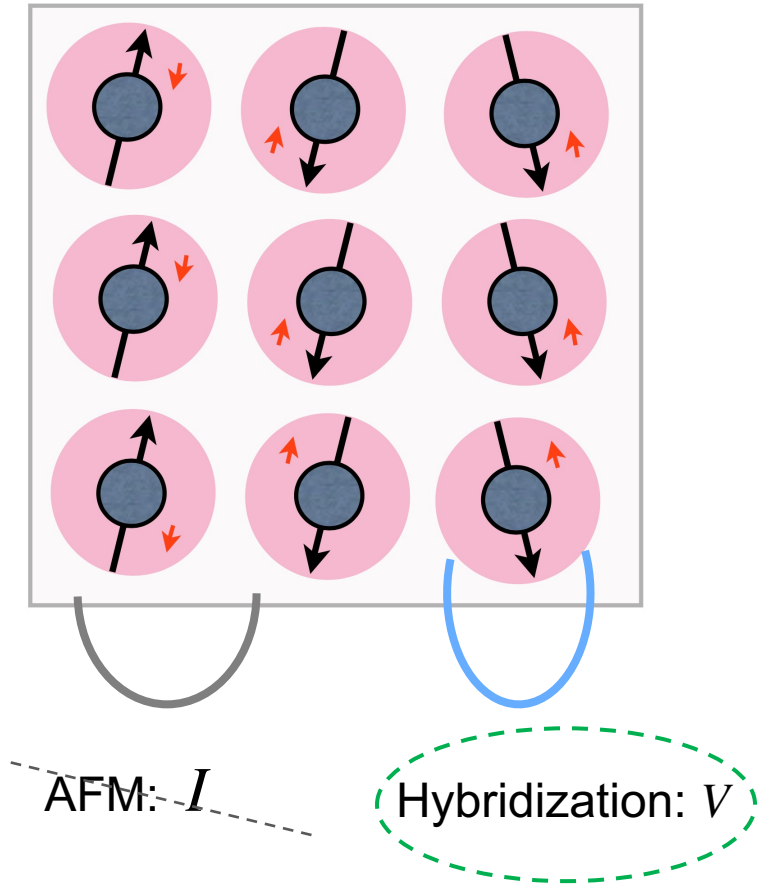
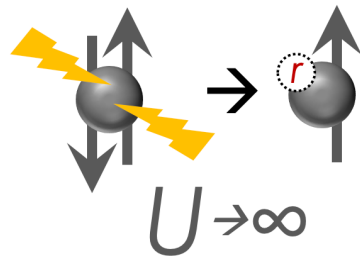
The Anderson lattice model

$$\mathcal{H} = \mathcal{H}_c + \mathcal{H}_{cd} + \mathcal{H}_d$$

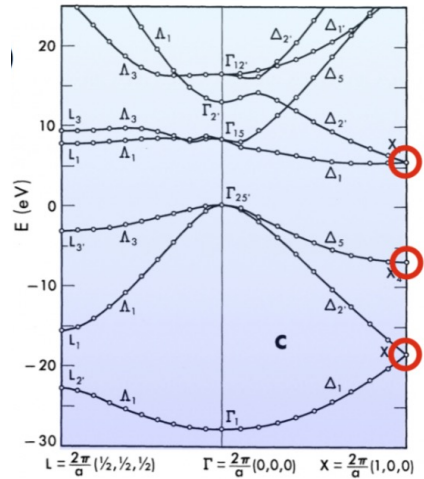
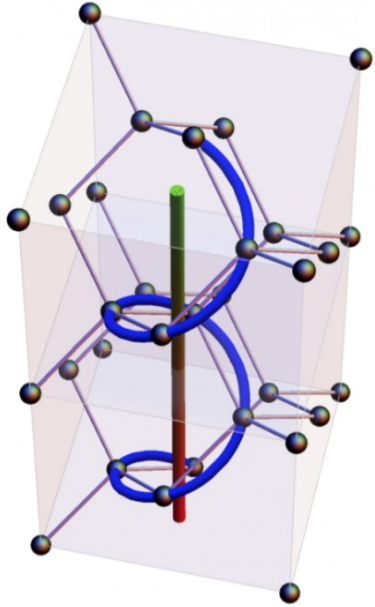
$$\mathcal{H}_{cd} = V \sum_{i,\sigma} \left(d_{i\sigma}^\dagger c_{i\sigma} + \text{H.c.} \right) \quad \text{hybridization}$$

$$\mathcal{H}_d = \sum_{i,\sigma} (E_d - \mu) d_{i\sigma}^\dagger d_{i\sigma} \quad \text{localized level}$$

$$+ U \sum_i n_{i\uparrow}^d n_{i\downarrow}^d \quad \text{Coulomb repulsion}$$



Conduction electrons



$$\mathcal{H}_c = t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.})$$

=nearest
neighbor
hopping

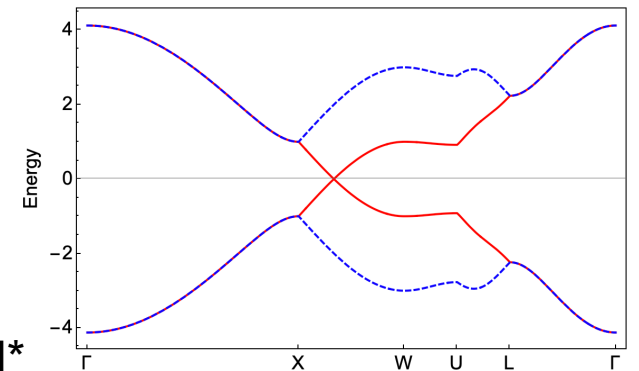
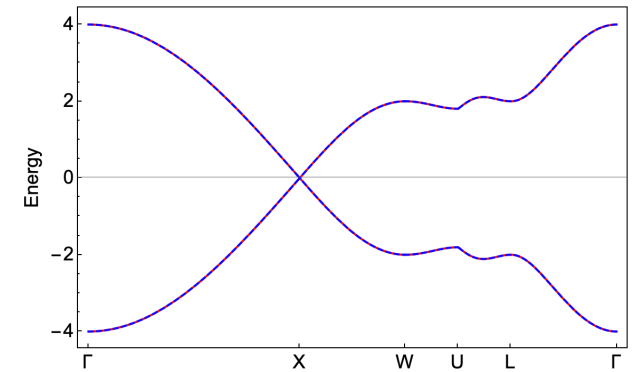
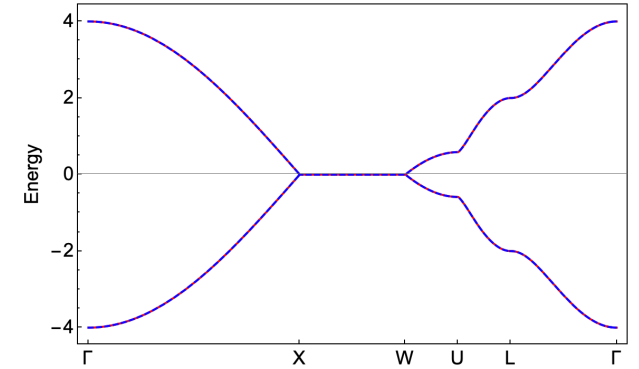
$$+ i\lambda \sum_{\langle\langle ij \rangle\rangle} [c_{i\sigma}^\dagger (\boldsymbol{\sigma} \cdot \mathbf{e}_{ij})_{\sigma\sigma'} c_{j\sigma'} - \text{H.c.}]$$

+spin-orbit
coupling

$$+ \sum_{i, \sigma} (m(-1)^i - \mu) n_{i\sigma}^c$$

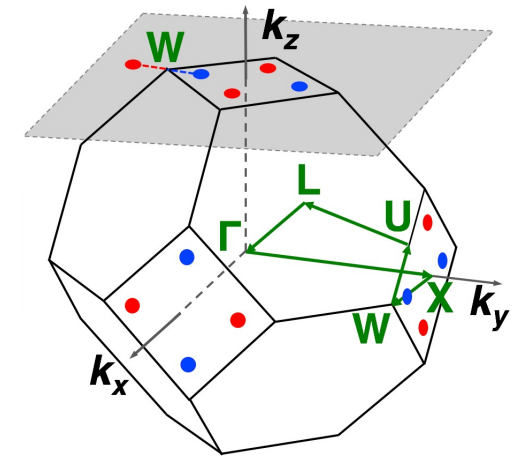
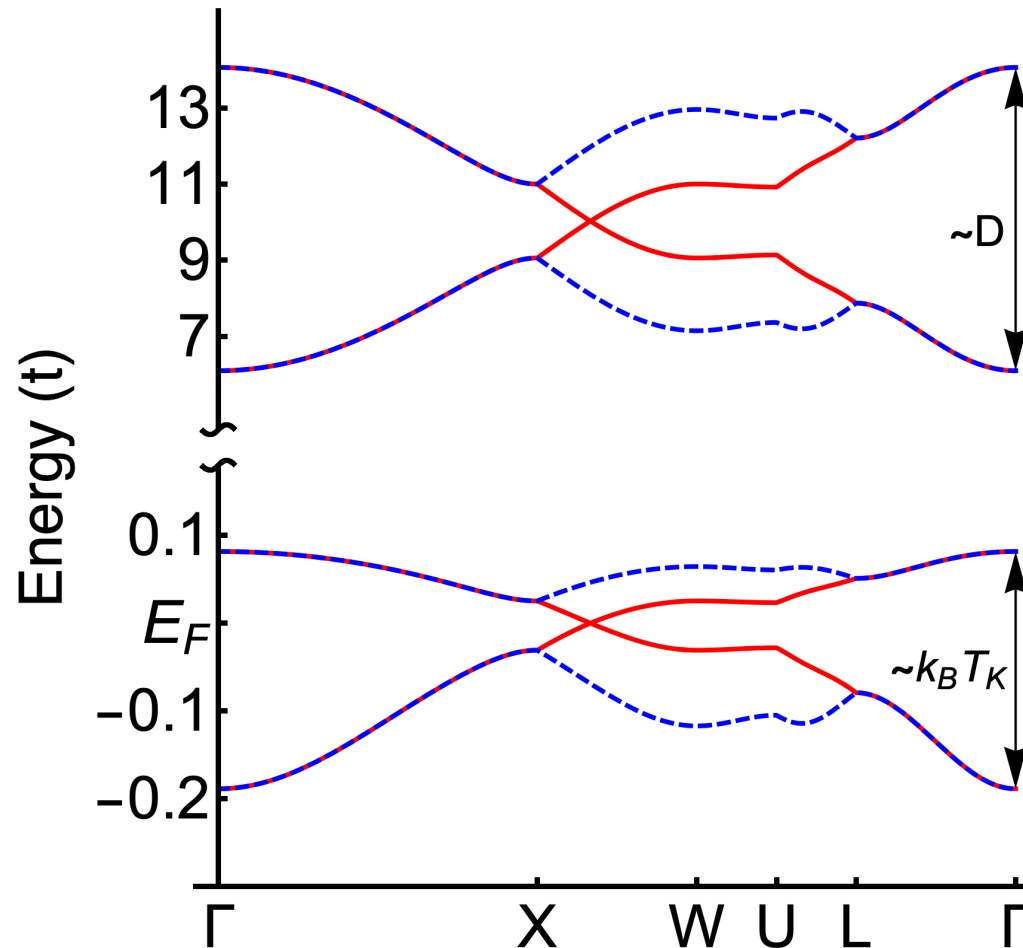
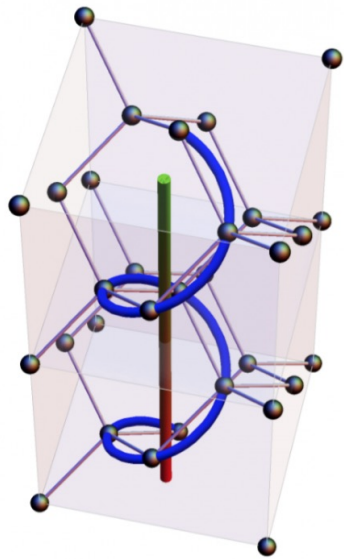
+break inversion
symmetry

= Weyl semimetal*



The Weyl-Kondo semimetal

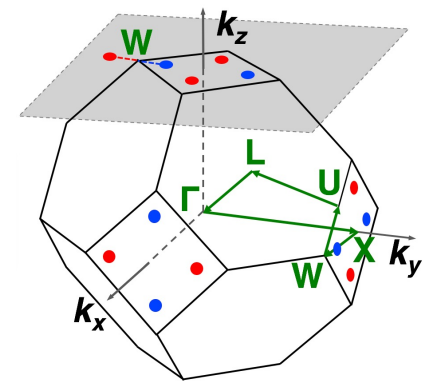
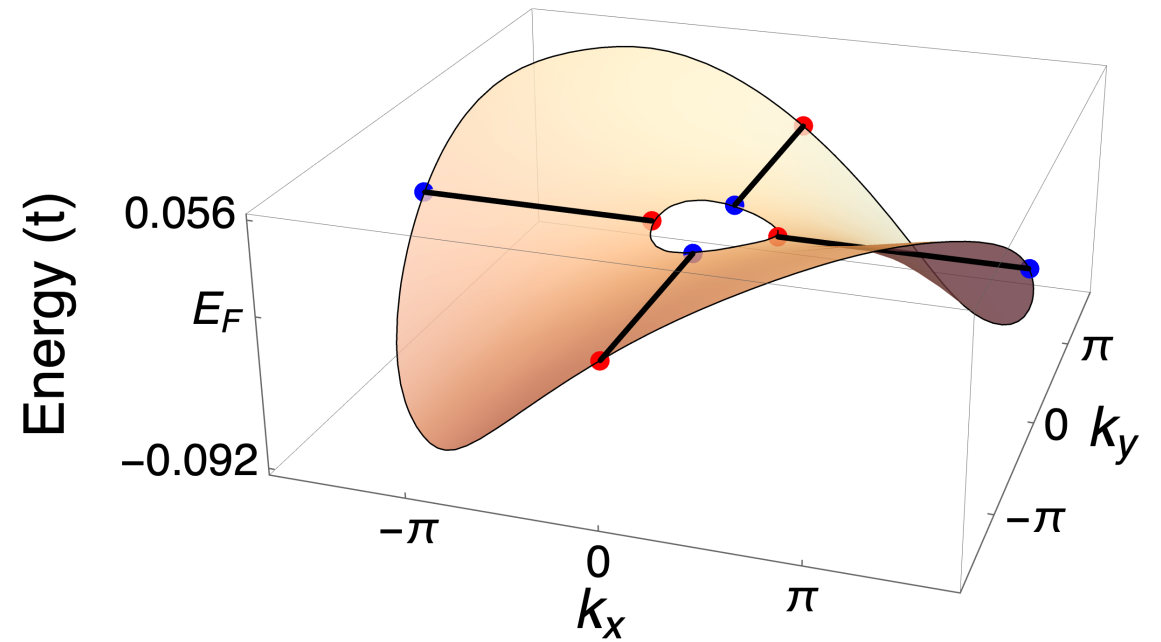
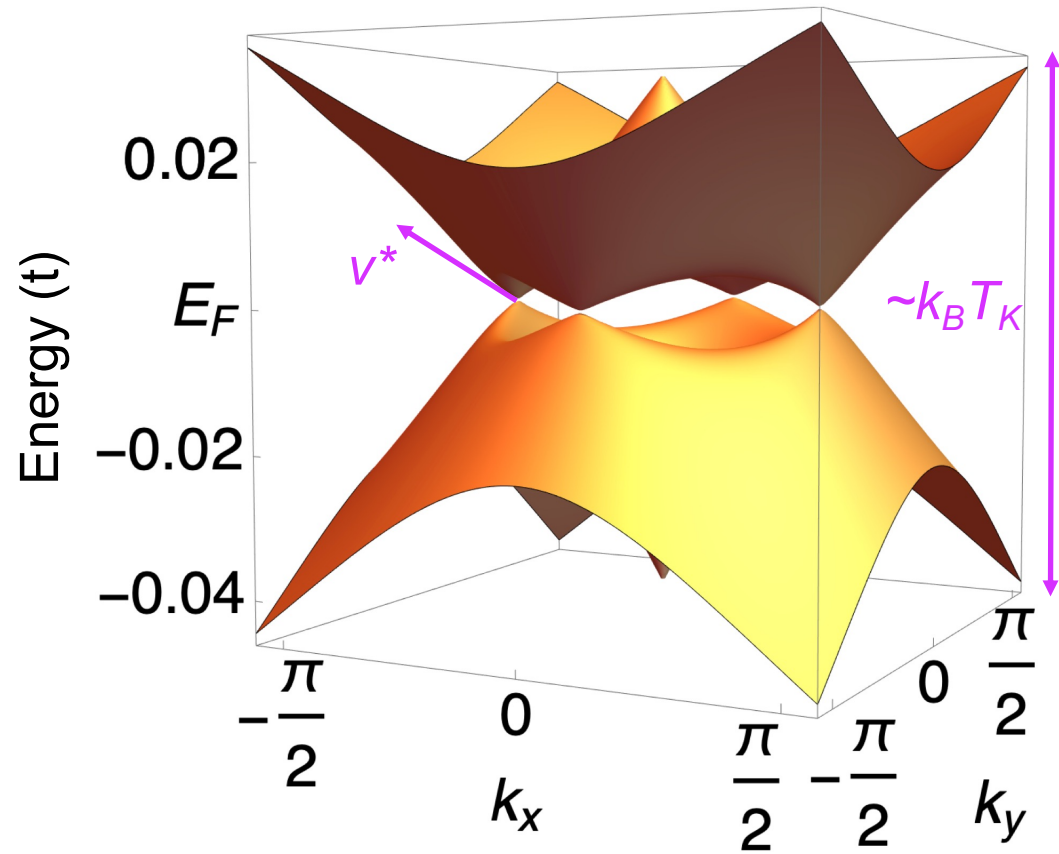
$$\mathcal{H} = \mathcal{H}_c + \mathcal{H}_{cd} + \mathcal{H}_d$$



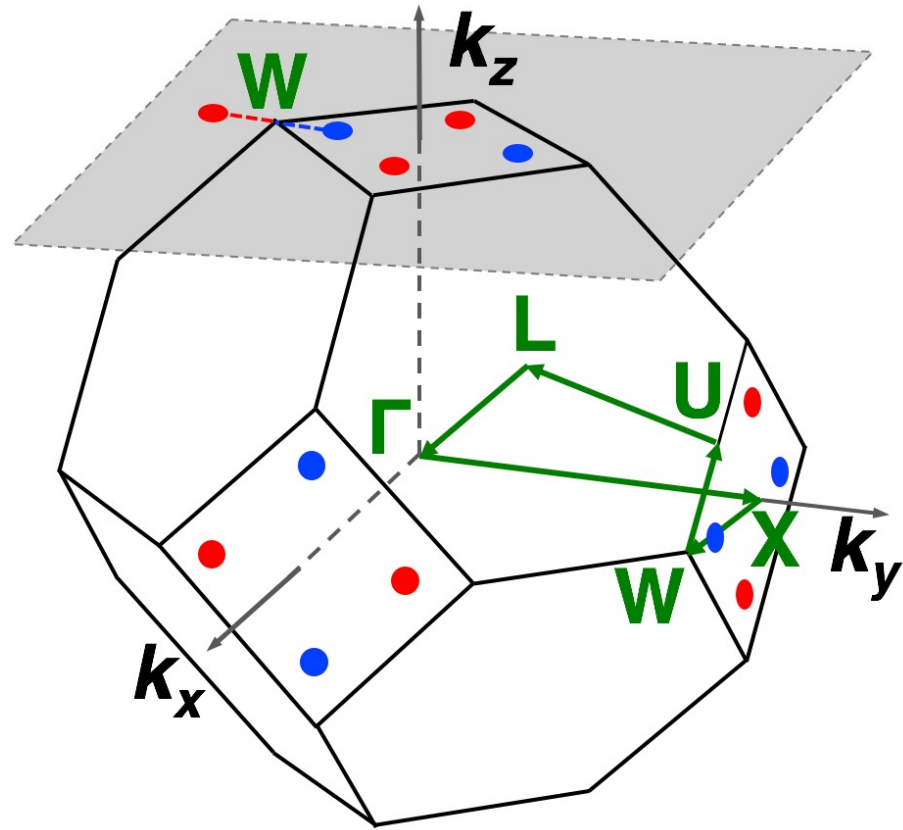
$$\hat{H} = \pm v_F^* \boldsymbol{\sigma} \cdot \mathbf{k}$$

- $D \gg k_B T_K$
- $v_F \gg v_F^*$
- Nodes at E_F

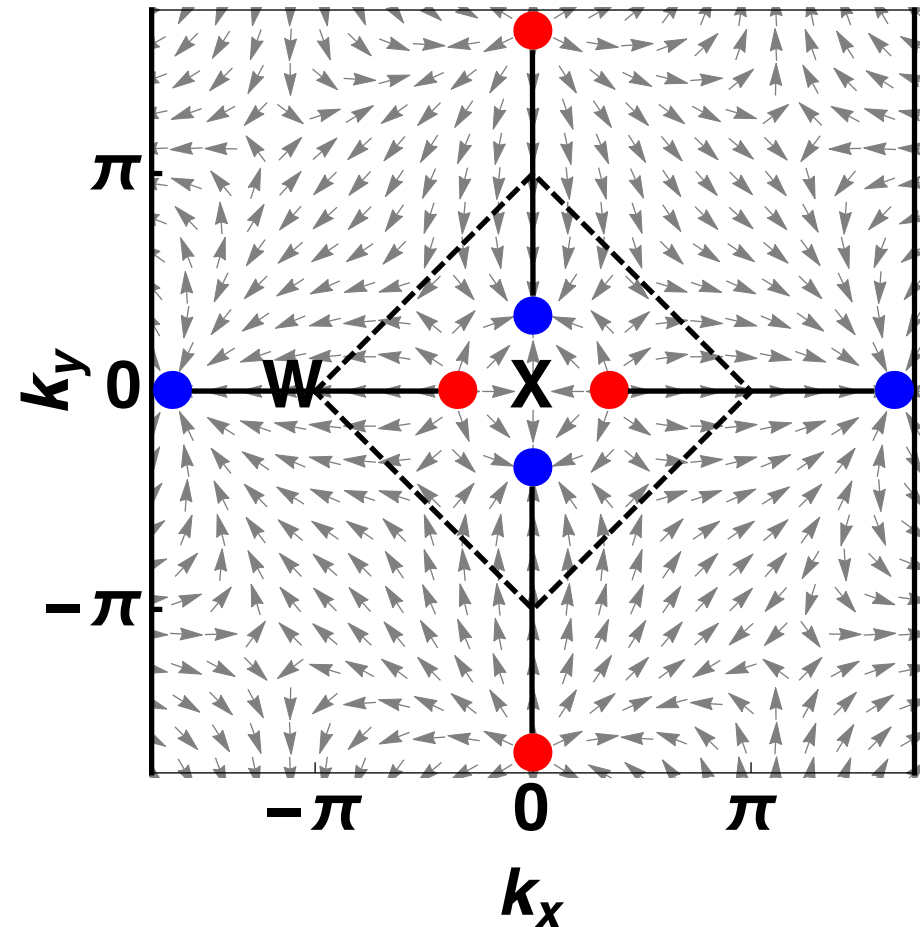
Bulk-surface correspondence



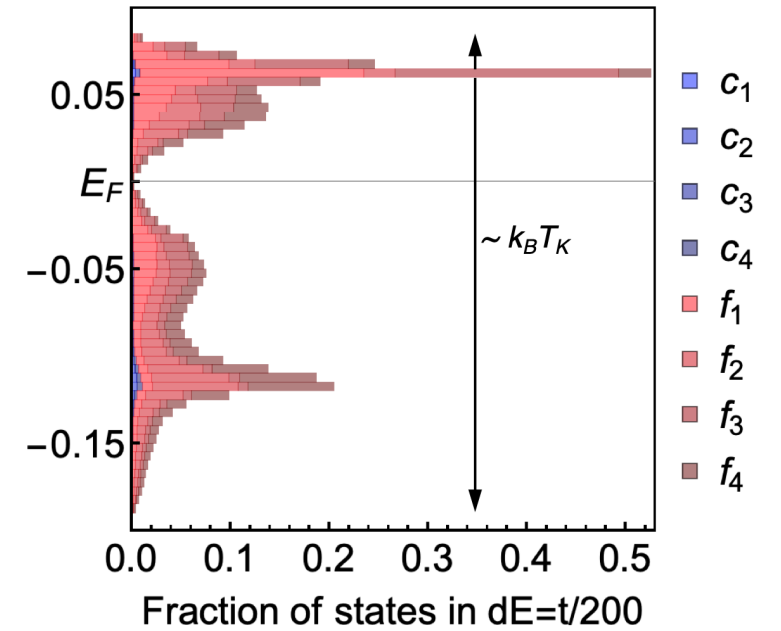
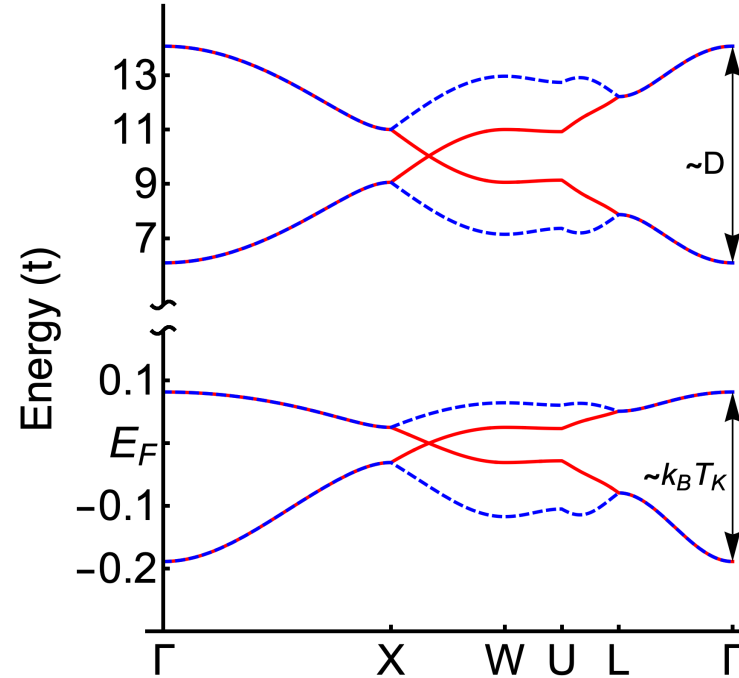
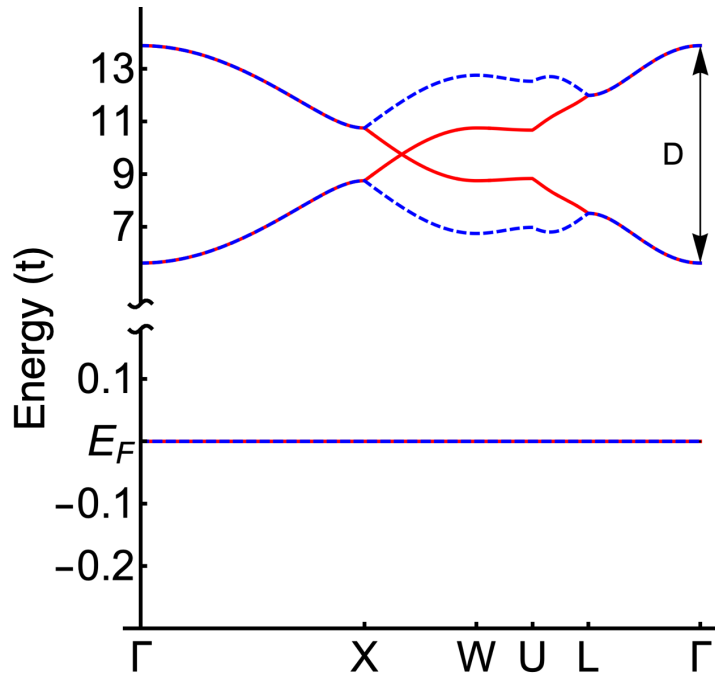
Topology and Berry curvature



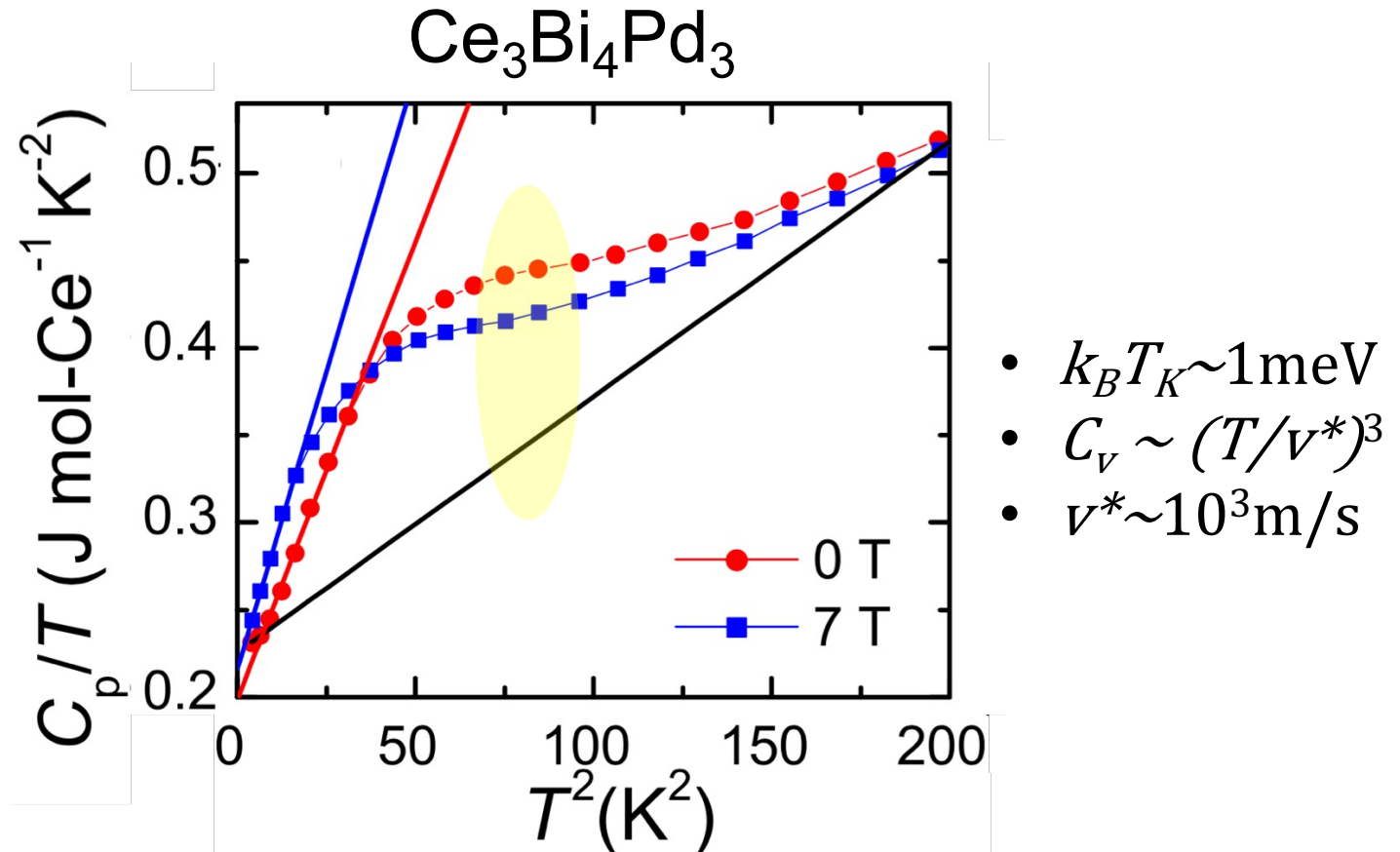
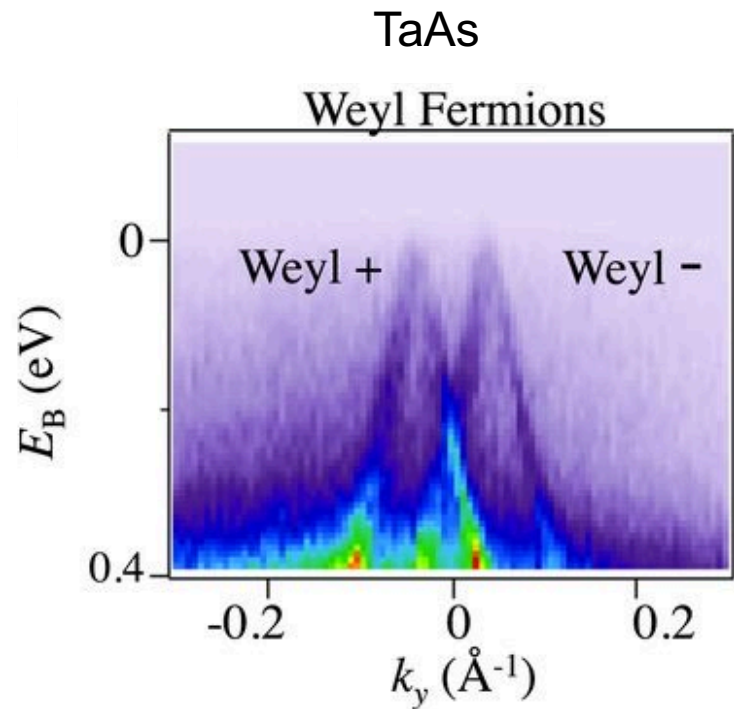
$$C_n = \frac{1}{2\pi} \int_{dS} \Omega_n(\mathbf{k}) \cdot d\mathbf{S} = \pm 1$$



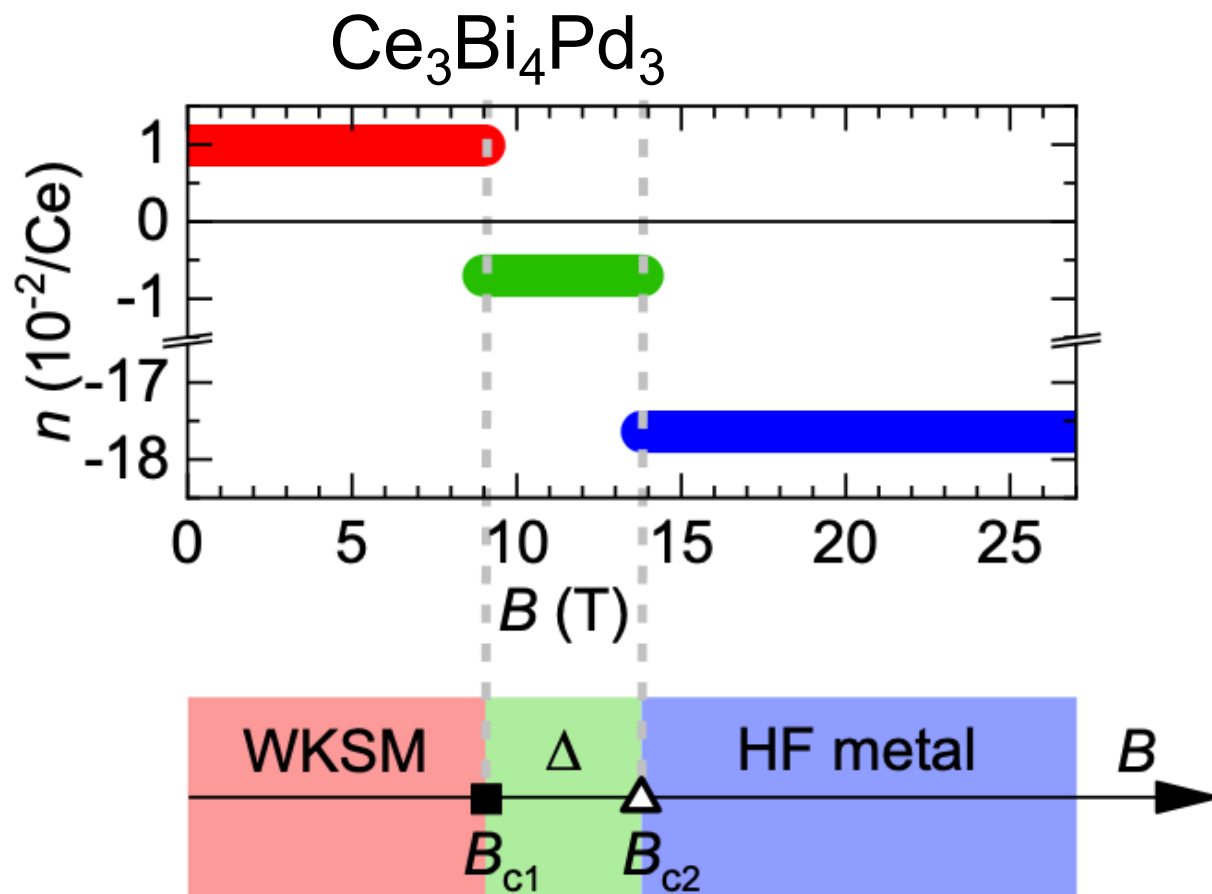
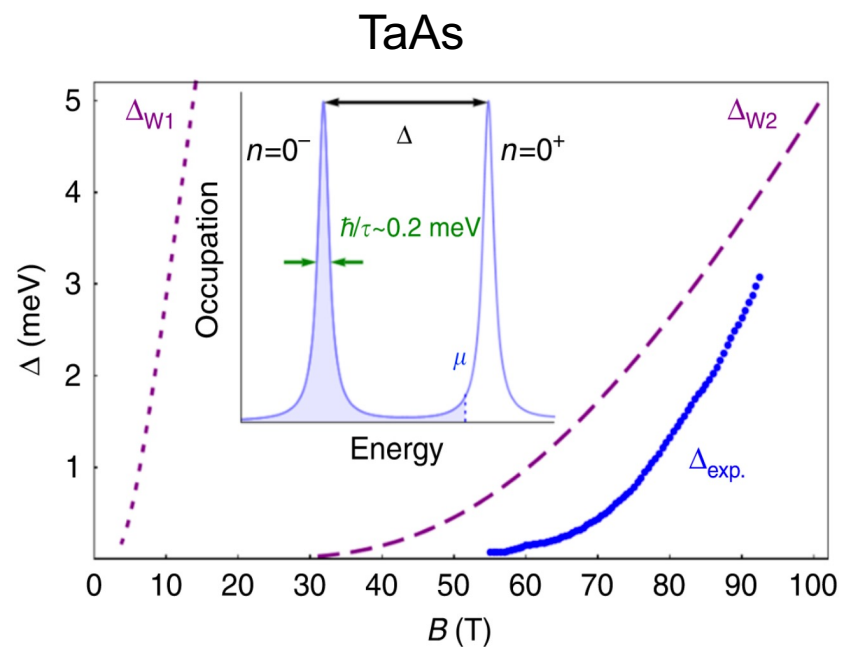
Kondo-pinning effect



Probing topology across correlation scales

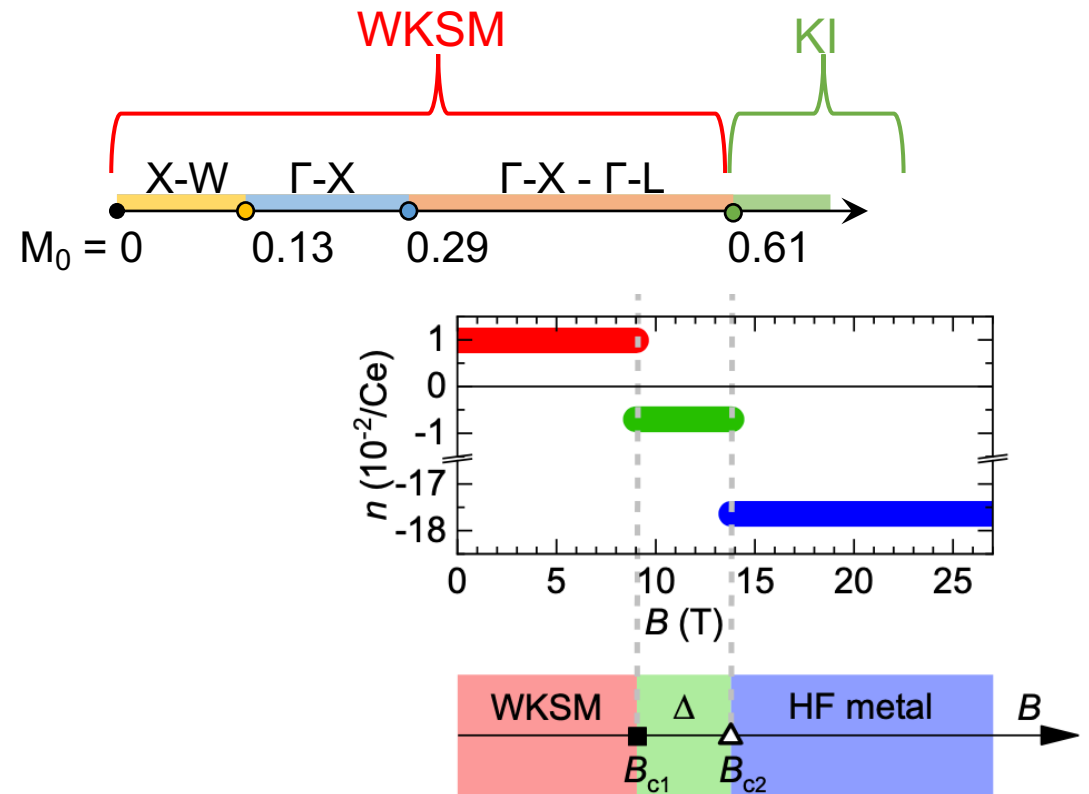
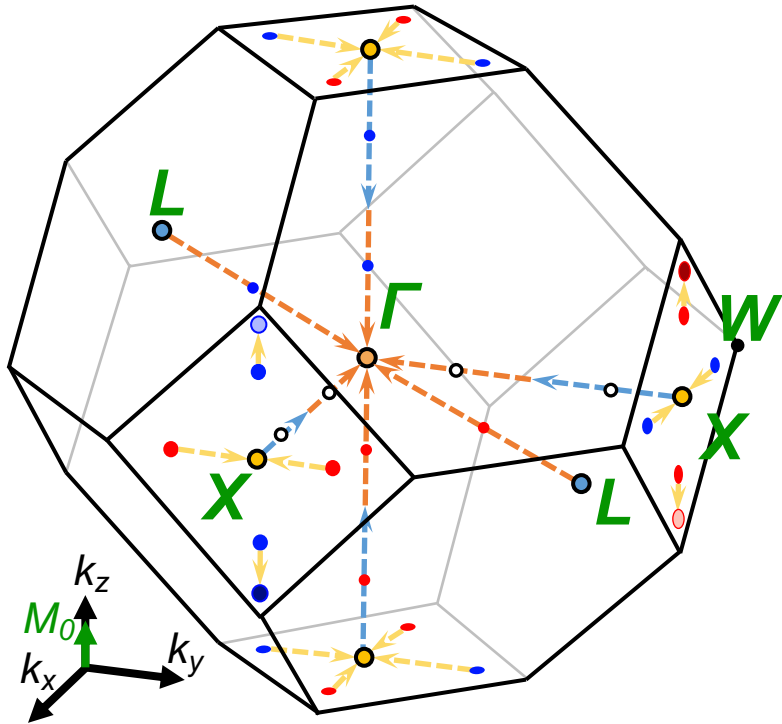


Probing topology across correlation scales



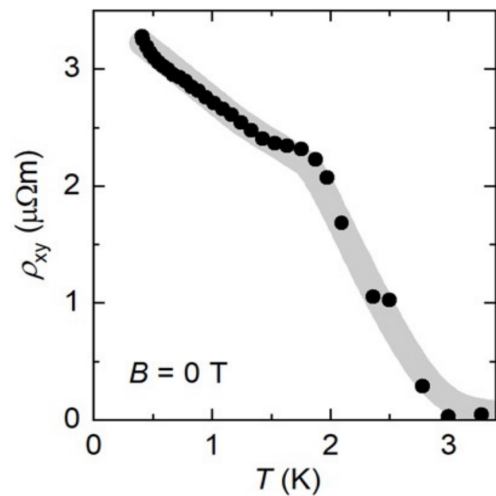
Correlations enable fine tuning

$$\mathcal{H} = \mathcal{H}_c + \mathcal{H}_{cd} + \mathcal{H}_d + M_0 \sum_{i,\sigma} \hat{z} \cdot (d_{i\sigma}^\dagger \vec{\sigma} d_{i\sigma})$$

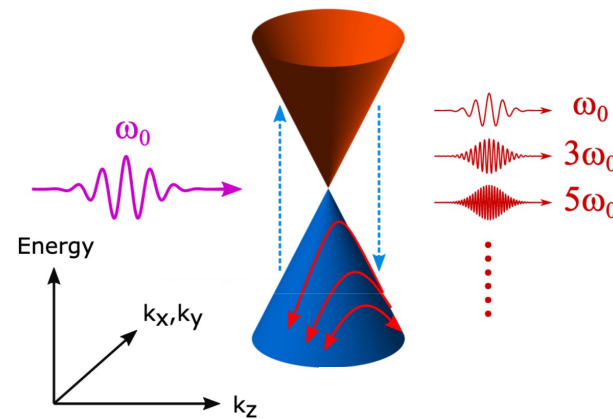


Ongoing and future projects

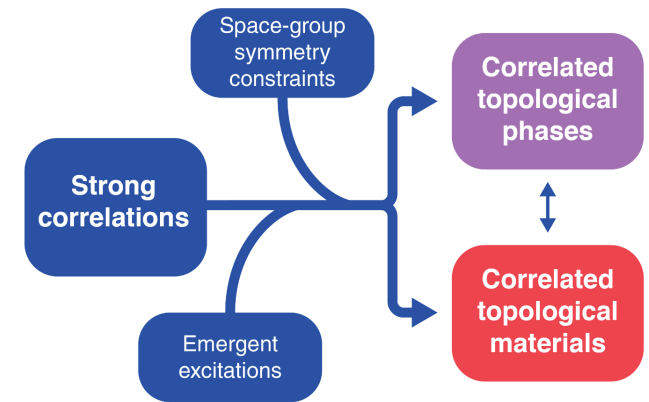
Nonequilibrium response



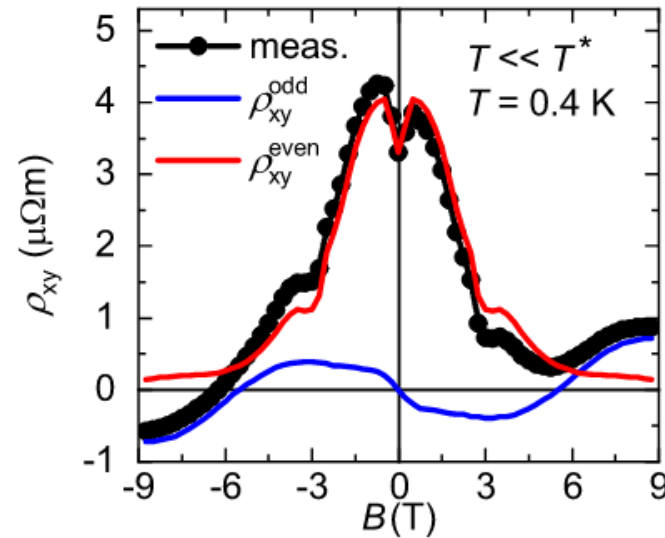
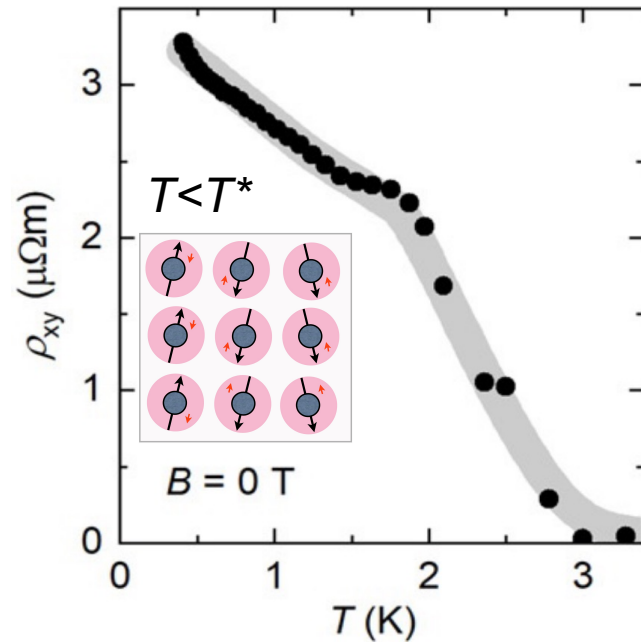
Nonlinear optical properties



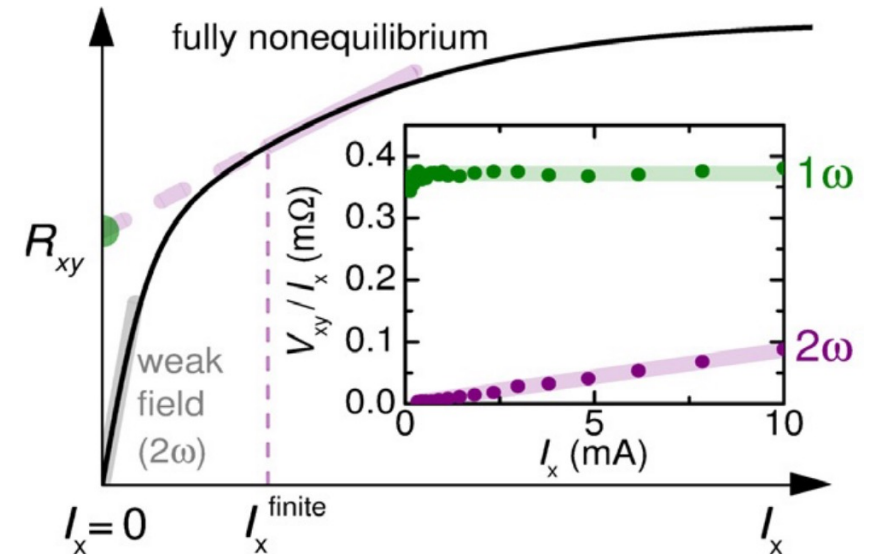
New models for applications



Giant topological Hall response



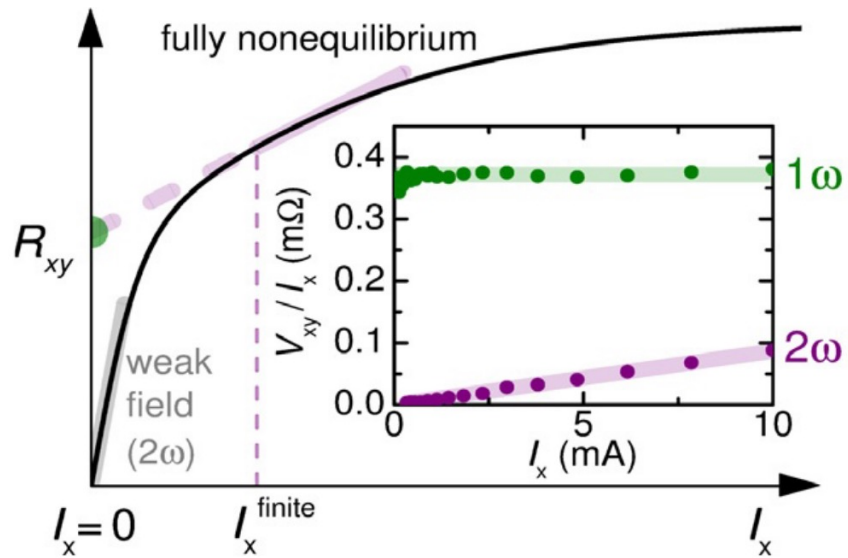
- ρ_{xy}^{odd} seen in TRSB WSMs
- ρ_{xy}^{even} consistent with $B=0$



$$2\omega: \sigma_{xy} = \frac{e^3 \tau}{\hbar^2} \cdot D_{xz} \cdot \mathcal{E}_x$$

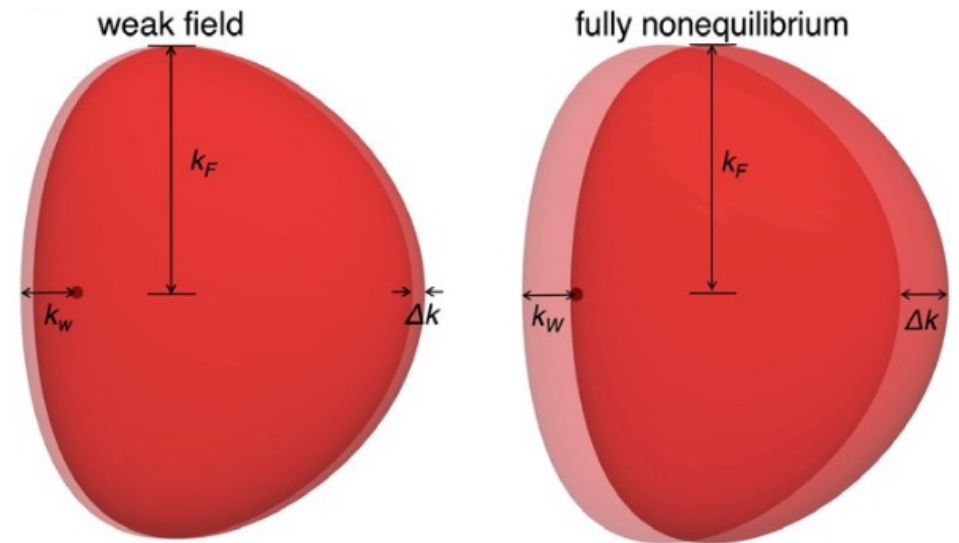
1 ω : ???

Fully nonequilibrium $\text{Ce}_3\text{Bi}_4\text{Pd}_3$



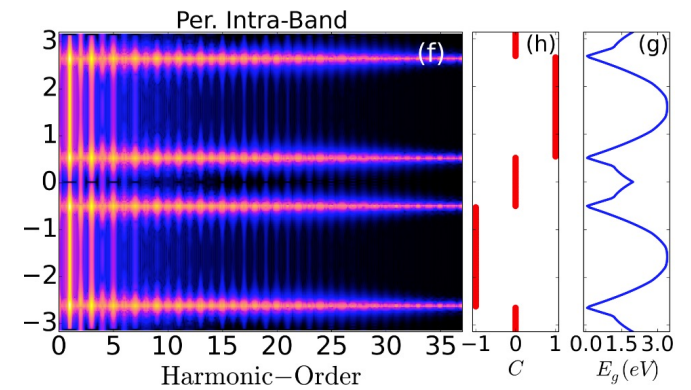
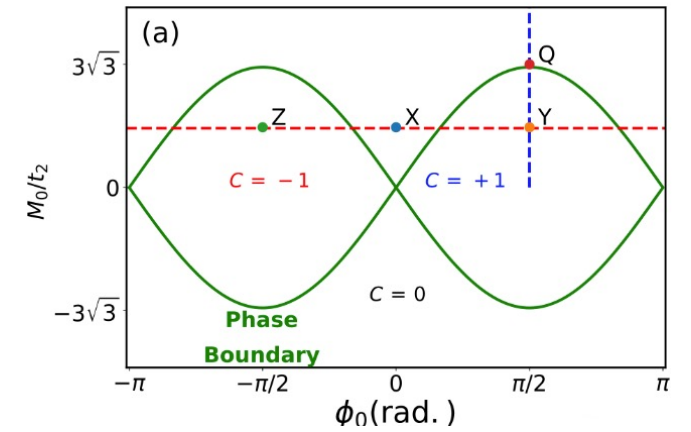
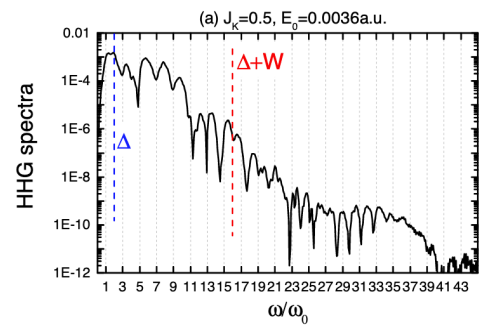
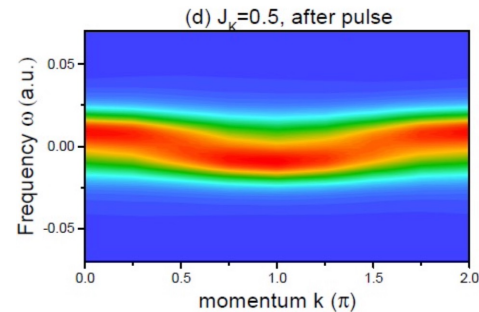
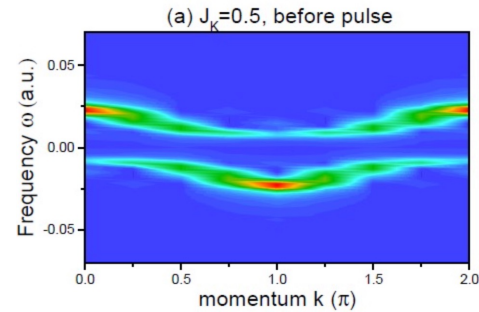
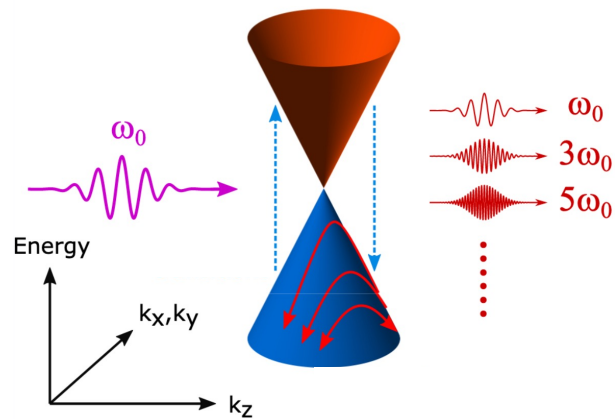
$$2\omega: \sigma_{xy} = \frac{e^3 \tau}{\hbar^2} \cdot D_{xz} \cdot \mathcal{E}_x$$

1ω : ???

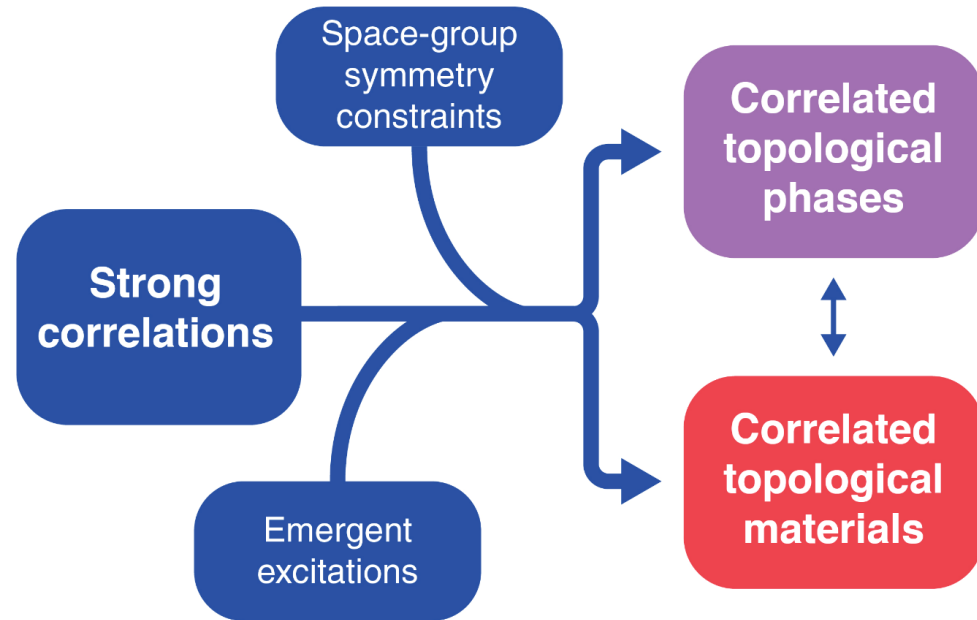
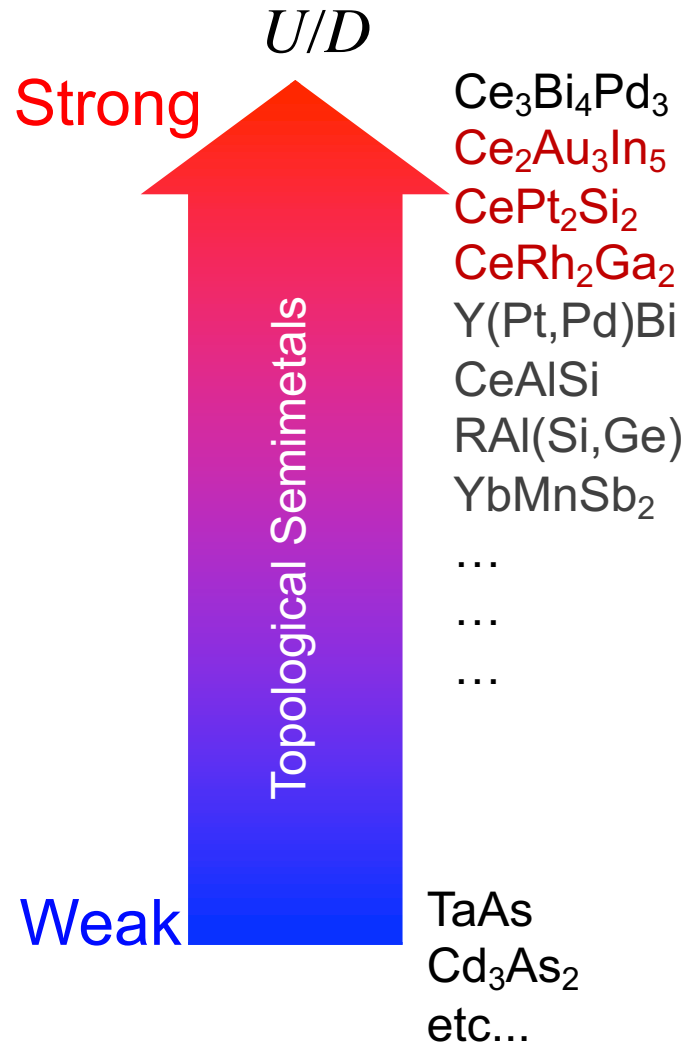


- $\mathbf{\Omega}(k_W)$ pinned close to Fermi surface
- Small electric fields \rightarrow fully nonequilibrium

High-harmonic generation

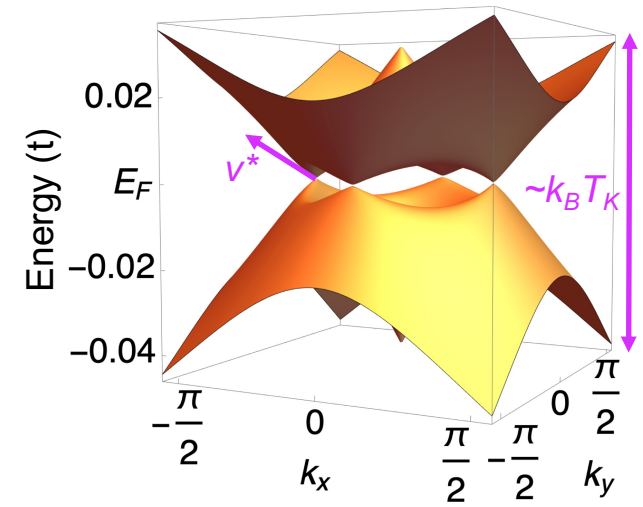
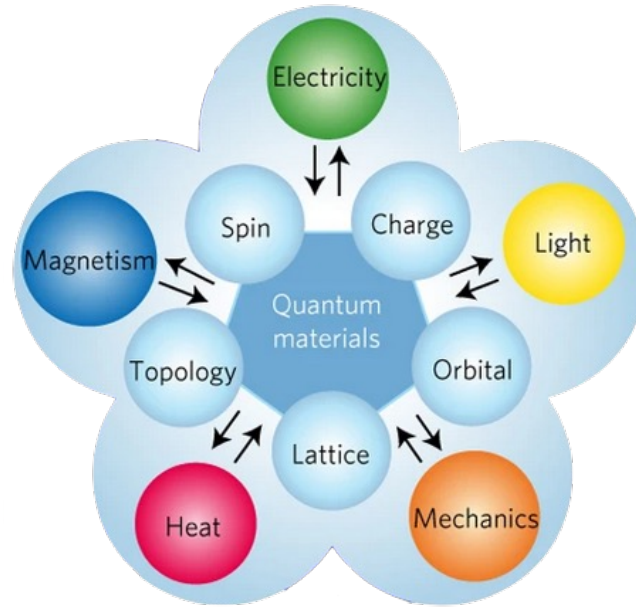
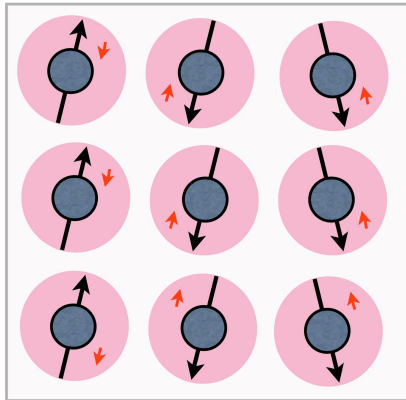
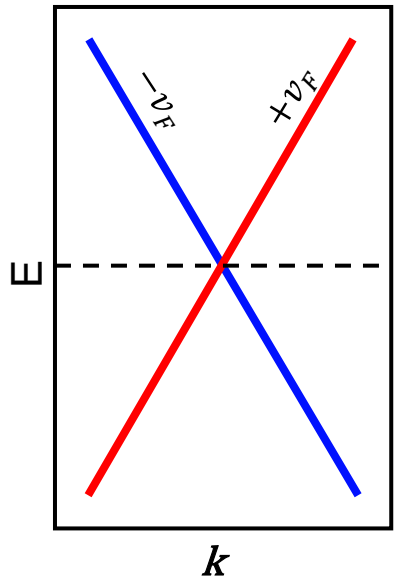


Strongly correlated topological semimetals



Symmetry-constrained emergent excitations

In conclusion...

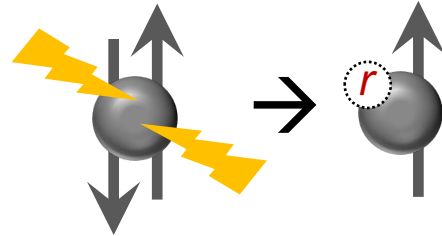


Auxiliary boson treatment

$$\mathcal{H}_{cd} = V \sum_{i,\sigma} \left(d_{i\sigma}^\dagger c_{i\sigma} + \text{H.c.} \right)$$

$$\mathcal{H}_d = \sum_{i,\sigma} (E_d - \mu) d_{i\sigma}^\dagger d_{i\sigma}$$

$$+ U \sum_i n_{i\uparrow}^d n_{i\downarrow}^d$$



$$\mathcal{H}_{cd} = rV \sum_{i,\sigma} \left(f_{i\sigma}^\dagger c_{i\sigma} + \text{H.c.} \right)$$

$$\mathcal{H}_d = \sum_{i,\sigma} (E_d - \mu) f_{i\sigma}^\dagger f_{i\sigma}$$

$$+ \ell \sum_{i,\sigma} (f_{i\sigma}^\dagger f_{i\sigma} + r^2 - 1)$$

- $U \rightarrow \infty$ Coulomb repulsion
 - enforces **1 f / site**
 - Treat hole fluctuations away from 1 as boson

$$U \rightarrow \infty$$

$$d_{i\sigma}^\dagger \rightarrow b_i f_{i\sigma}^\dagger$$

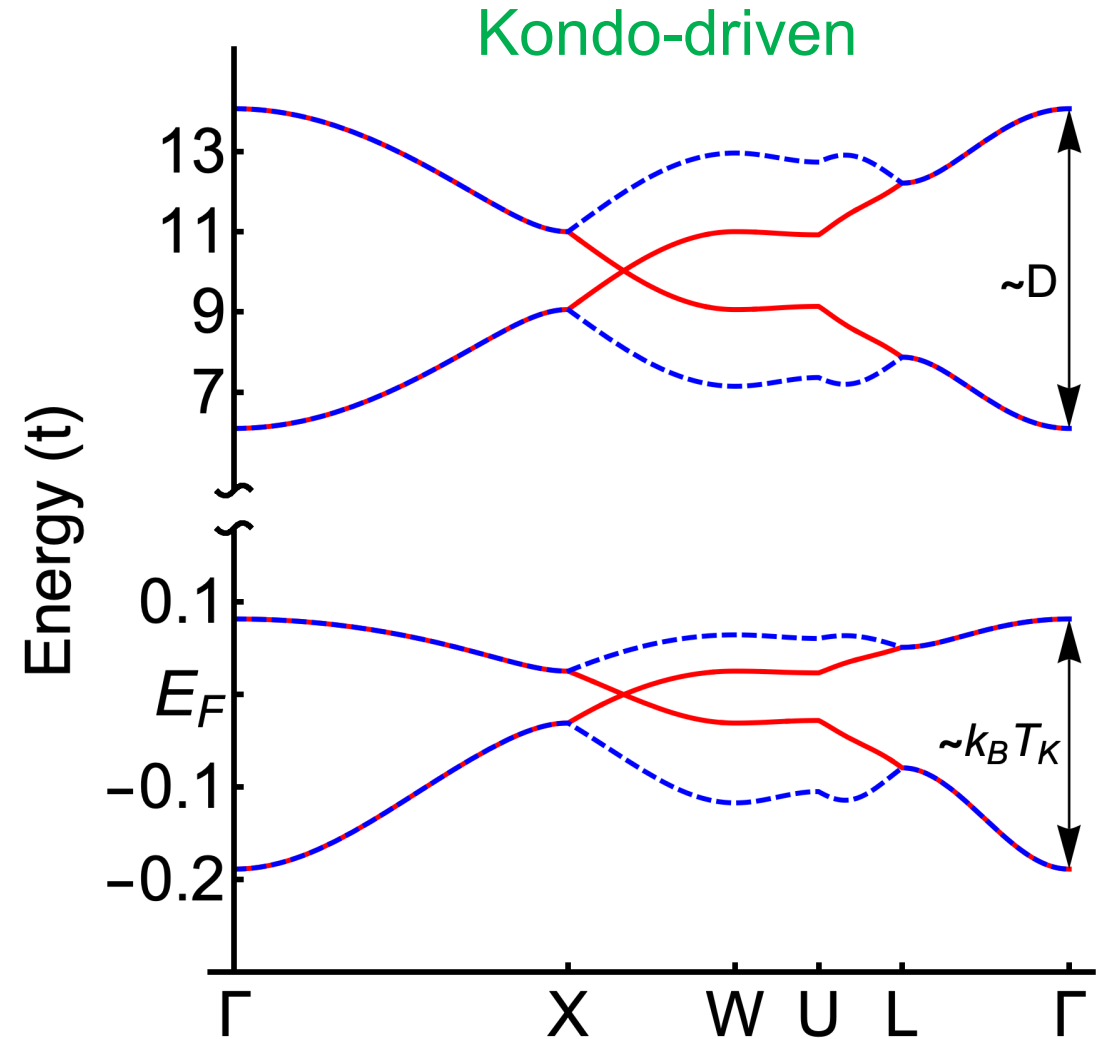
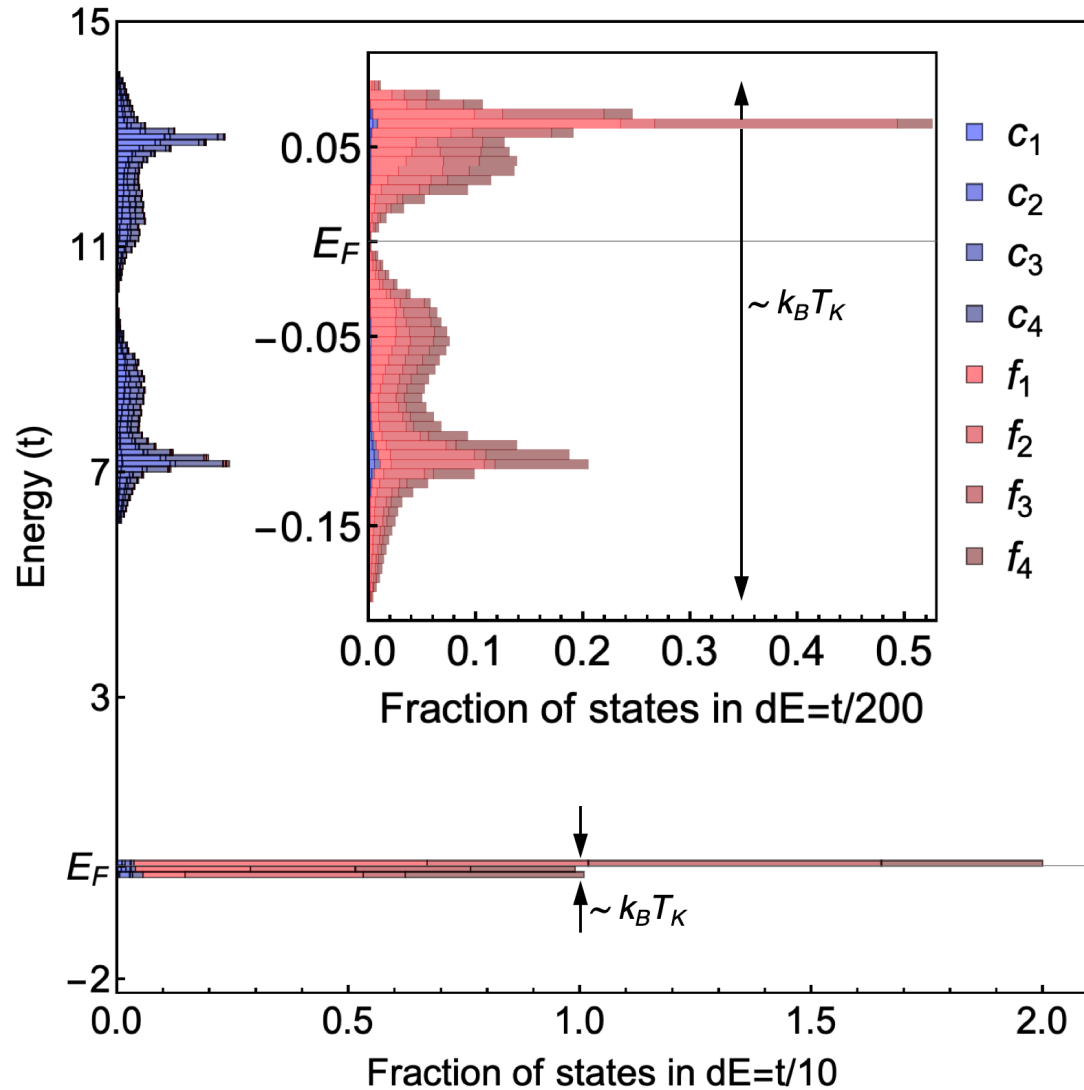
$$b_i \rightarrow \langle b_i \rangle = r$$

$$\sum_{i,\sigma} f_{i\sigma}^\dagger f_{i\sigma} + r^2 = 1$$

$$n_{tot} = n_d + n_c$$

Crystal symmetry + topology:
Gaplessness guaranteed at n-odd-quarter fillings: $n/(\text{spin per unit cell})$

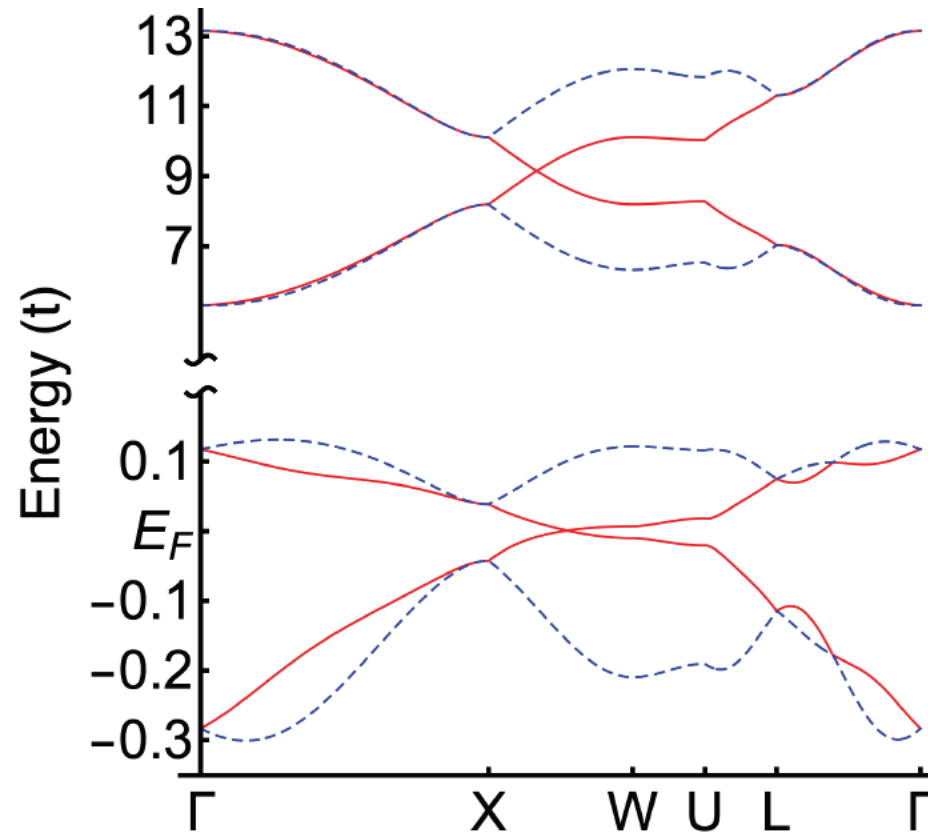
Weyl-Kondo semimetal properties



Weyl-Kondo semimetal with spin-orbit coupling hybridization

- SOC between f and c species
- Quarter filling
 - $n_c+n_d=1$ per site

SEG, H. H. Lai, S. Paschen & Q. Si, in preparation.



Zeeman field: uncorrelated model

Conduction electron-only model

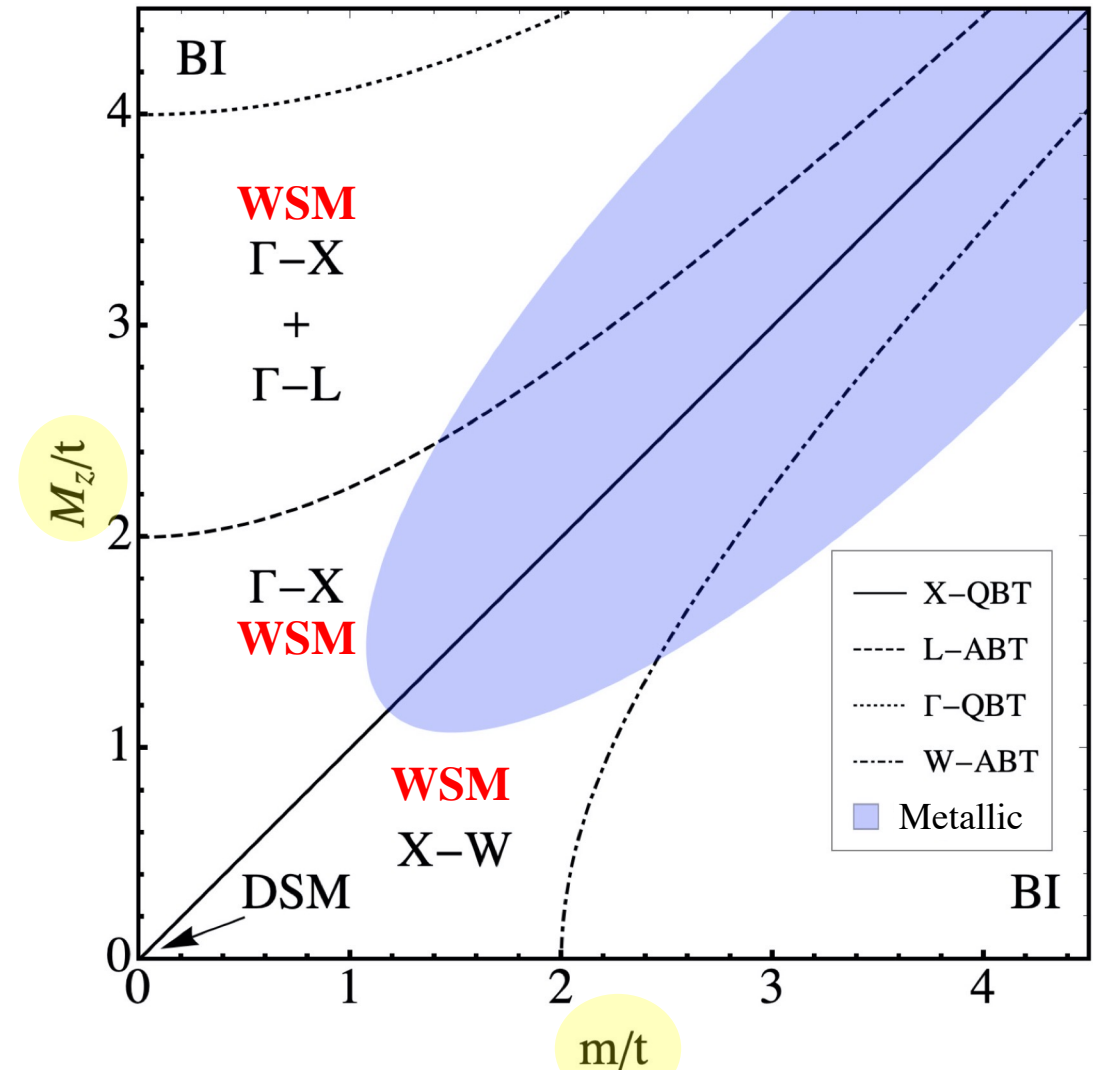
- Diamond crystal structure

$$\mathcal{H}_c = \sum_{\langle ij \rangle, \sigma} \left(t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.} \right) - \mu \sum_{i, \sigma} n_{i\sigma}^c$$

$$+ m \sum_{i, \sigma} (-1)^i c_{i\sigma}^\dagger c_{i\sigma} + M_z \sum_j \hat{z} \cdot (c_{j\sigma}^\dagger \boldsymbol{\sigma} c_{j\sigma})$$

$$+ i\lambda \sum_{\langle\langle ij \rangle\rangle} \left[c_{i\sigma}^\dagger (\boldsymbol{\sigma} \cdot \mathbf{e}_{ij}) c_{j\sigma} - \text{H.c.} \right],$$

- Hopping (t) & chemical potential
- Inversion symmetry breaking, m/t
- Zeeman exchange field, M_z/t
- Spin-orbit coupling



Peierls treatment and current

- Light pulse – vector potential field

$$\mathbf{A}(t) = (A_x(t), A_y(t), A_z(t))$$

- Pulse envelope

$$A_i = 2\pi A_{i0} \exp\left(-\frac{(t-t_c)^2}{2t_d^2}\right) \cos(\omega(t-t_c))$$

- Operators get phase factor

$$c_{i\sigma}^\dagger \rightarrow c_{i\sigma}^\dagger \exp\left(\frac{ie}{\hbar c} \int_{\mathbf{R}_\infty}^{\mathbf{R}_i} d\mathbf{R} \cdot \mathbf{A}(t)\right)$$

- Only kinetic (hopping) terms affected

$$t \rightarrow t \exp\{-i\mathbf{A}(t) \cdot (\mathbf{R}_i - \mathbf{R}_j)\} \quad \frac{e}{\hbar c} = 1$$

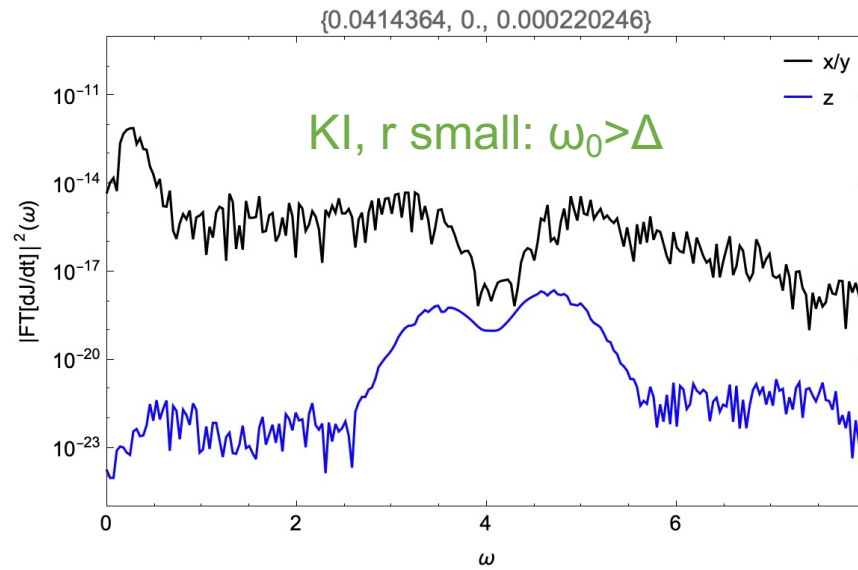
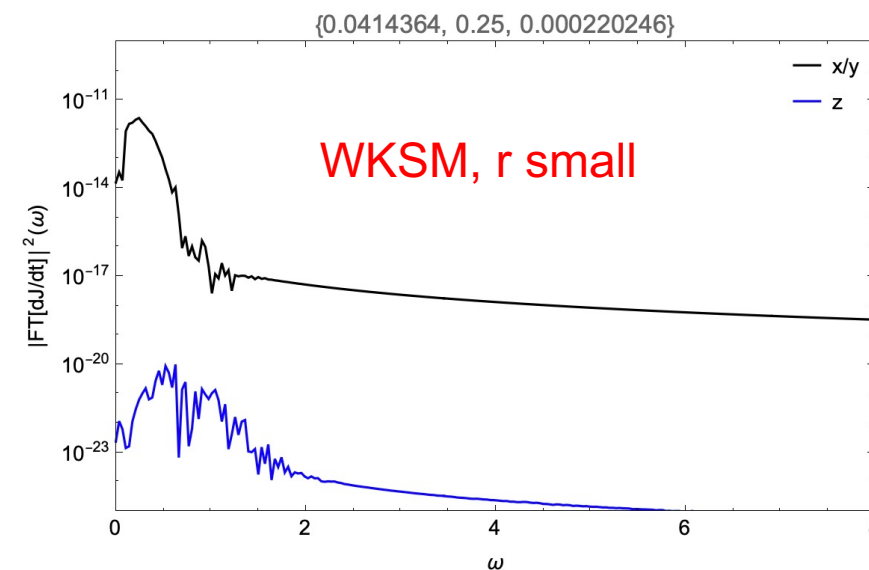
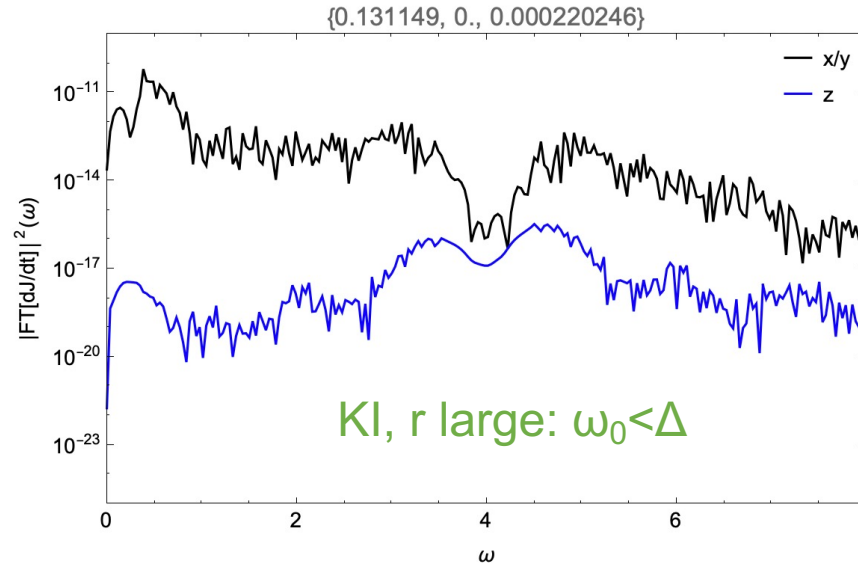
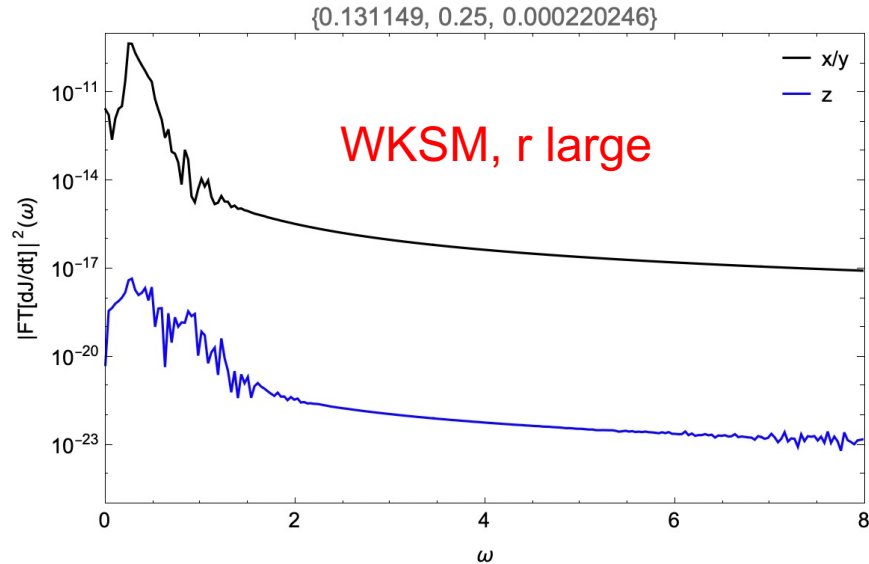
$$\lambda \rightarrow \lambda \exp\{-i\mathbf{A}(t) \cdot (\mathbf{R}_i - \mathbf{R}_j)\}$$

- Generalized current expression that contains all harmonic orders:

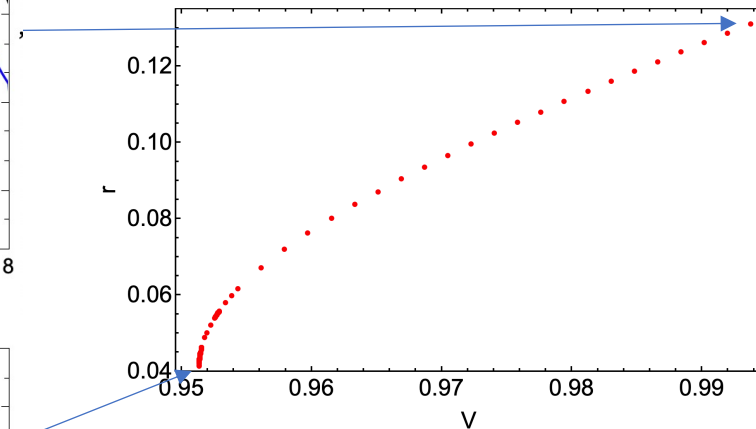
$$\langle \vec{J}(t) \rangle = \frac{e}{V_\Omega N_L \hbar} \sum_{n\mathbf{k}} \sum_{i,j} v_{ij}(\mathbf{k}, t) \phi_{in}^*(\mathbf{k}, t) \phi_{jn}(\mathbf{k}, t) f[-E_n(\mathbf{k}, t)]$$

$$v_{ij}(\mathbf{k}, t) = \sum_{\nu} (\mathbf{R}_\nu + \mathbf{r}_{\tau'} - \mathbf{r}_{\tau'}) h_{\tau\alpha, \tau'\beta}(\mathbf{k}, t) e^{i(\mathbf{k} - \vec{A}(t)) \cdot \mathbf{R}_\nu}$$

HHG: WKSM vs. KI



- Contrasting high harmonic response
- Both: smaller $r \rightarrow$ stronger renormalization \rightarrow signal weaker
- WKSM: low ω , linear dispersion
- KI: interband, $n\omega$



- Future work:
 - More realistic model systems
 - Compare with totally uncorrelated models
 - Energy-momentum resolved spectra
 - ...