Title: Interactions and Spin Orbit: from Weyls to Helical Spin Liquids

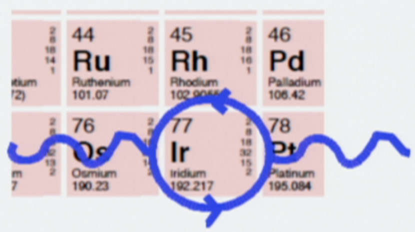
Date: Dec 08, 2011 02:00 PM

URL: http://pirsa.org/11120075

Abstract: Novel phases can result from the interplay of electronic interactions and spin orbit coupling. In the first part, we discuss a simple Hubbard model for the pyrochlore iridates, whose phase diagram contains topological insulator (TI) and various magnetic phases. The latter host the novel topological Weyl semimetal, whose excitations behave like Weyl fermions. In the second part we study a novel spin liquid that was proposed to arise in the iridates, the 3D topological Mott insulator: a fractionalized TI where the neutral spinons acquire a topologically non-trivial band structure. The low-energy behavior is dominated by the 2D surface spinons strongly coupled to a bulk gauge field. This phase is characterized by the helical nature of the spinon surface states and the dimensional mismatch between the latter and the gauge bosons. We discuss experimental signatures as well as the possibility of dyonic excitations and a non-trivial magneto-electric response.

Interplay of interactions and SO coupling: from **Weyls** to **helical spin liquids**

William Witczak-Krempa
University of Toronto, Canada



UNIVERSITY OF TORONTO

Fonds de recherche
Nature et
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Québec

Walter Sumner
Foundation

NSERC
CRSNG

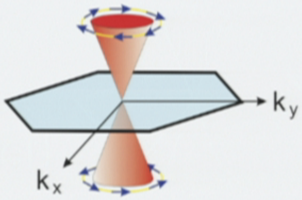
Overview

- Intro (TI, pyrochlore iridates)
- Topological & magnetic phases in the iridates
  - Effective microscopic Hamiltonian
  - MFT & Strong coupling
  - C-DMFT
- Topological Mott insulator
  - Slave-rotors & MFT by Pesin/Balents
  - Effect of gauge fluctuations
  - Non-quantized ME response, dyons?

Topological (band) insulators

- Are all 3D TRS band insulators the same?
  NO!
  Theory: Fu, Kane & Mele 2007; Moore & Balents 2007; Roy 2009. Exp: Hsieh et al. 2008
- Z_2 classification: $(\nu_0, \nu_1\nu_2\nu_3)$ $\nu_i = 0$ or 1
- $\nu_0 = 1$: **strong topological insulator** (TI, TBI)

Special surface states:
1) Odd number of Dirac cones
2) Robust to non-mag disorder!



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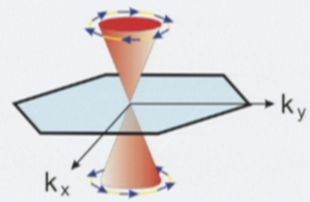
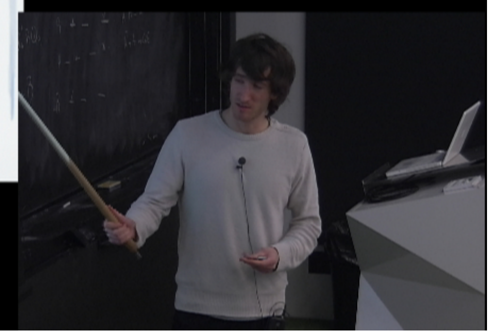
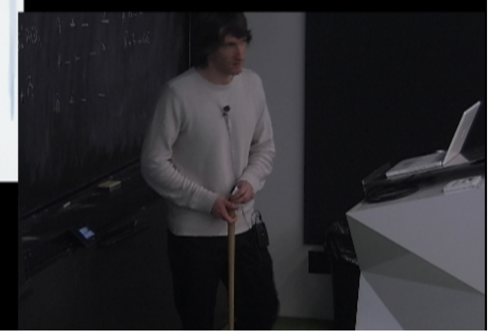




Interactions in TIs

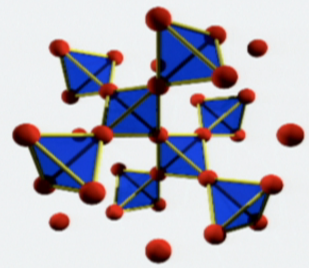
- 2 possibilities:
  - Qualitatively the same (weak/moderate corr)
  - Not connected to TBI

- Experimental candidates



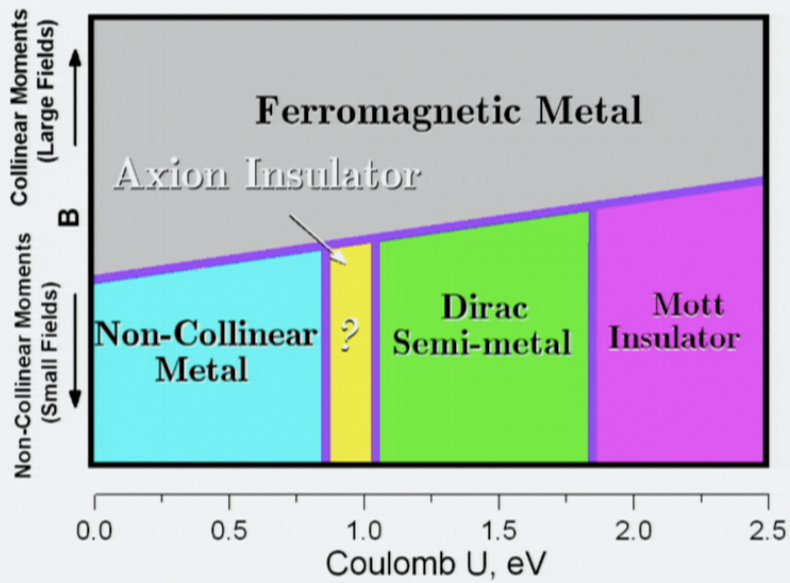
Pyrochlore Iridates

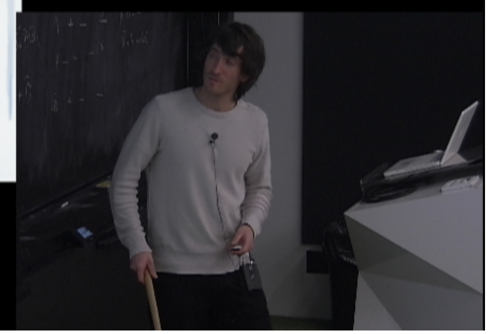
- Motivation: **Strong SO + Correlations = ?**
- Transition metal oxides: $A_2\mathrm{Ir}_2\mathrm{O}_7$
  A = Y or Lanthanide
- A & Ir: pyrochlore lattice
- Key physics → Ir^{4+}: $5d^5$
- Experiments
  - MIT as apply chemical or physical P
  - Hints of magnetic order (muSR)
- Theory: TI and novel SL (Pesin & Balents)



Ab initio

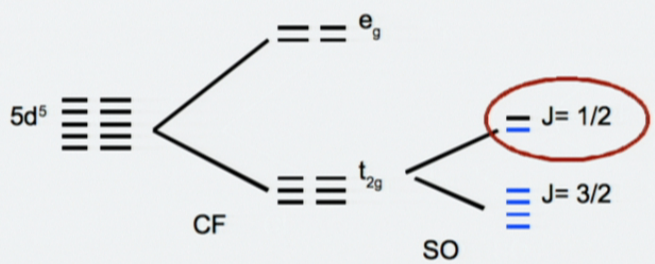
(Wan et al., PRB 2011)





Microscopic model

(WWK & Y. B. Kim, arXiv:1105.6108.)



- Focus on Ir, i.e. non magnetic A-site
- Pseudospin J_{eff} = 1/2

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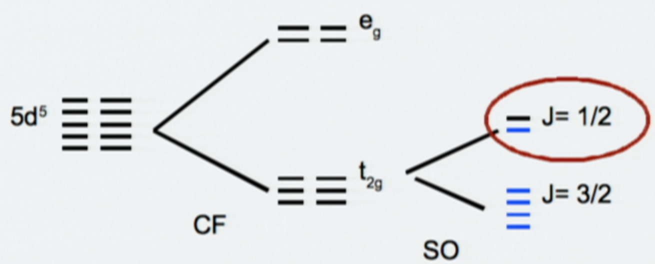

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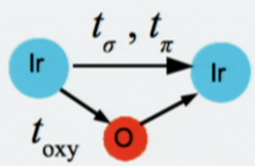
Microscopic model

- 2 hopping channels b/w NN Ir's
  - Oxygen mediated [Pesin & Balents]
  - Direct overlap



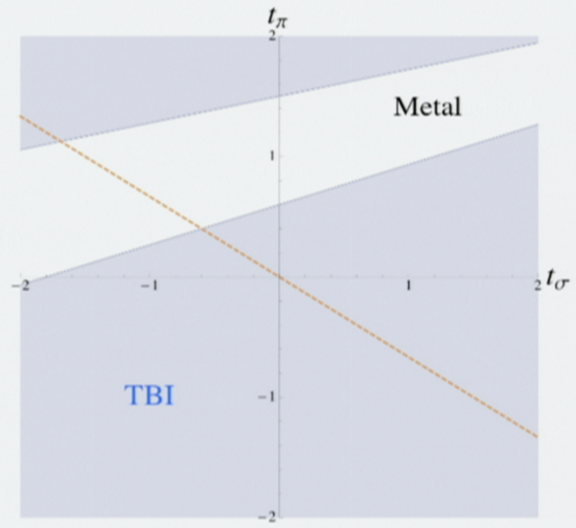
- Hubbard repulsion b/w electrons on Ir

$$H_0 = \sum_{\langle Ri, R'i' \rangle, \alpha\alpha'} (T^{ii'}_{\text{oxy},\alpha\alpha'} + T^{ii'}_{\text{d},\alpha\alpha'}) d^\dagger_{Ri\alpha} d_{R'i'\alpha'}$$

$$\boxed{H_U = U \sum_{Ri} n_{Ri\uparrow} n_{Ri\downarrow}}$$

$U = 0$ phase diagram

Hoppings
- $t_{oxy} = 1$
- $t_\sigma, t_\pi \rightarrow$ direct hop



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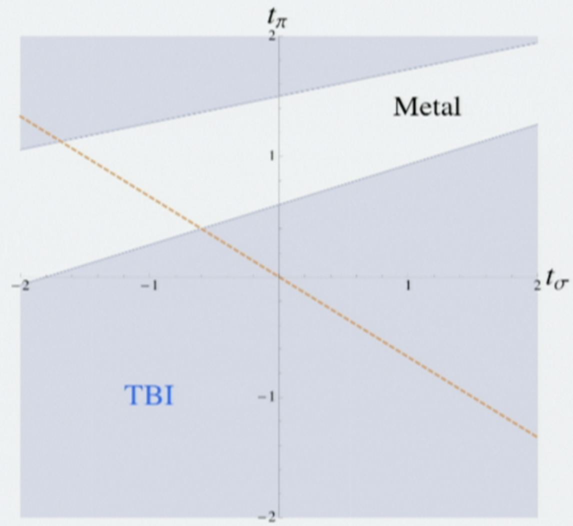
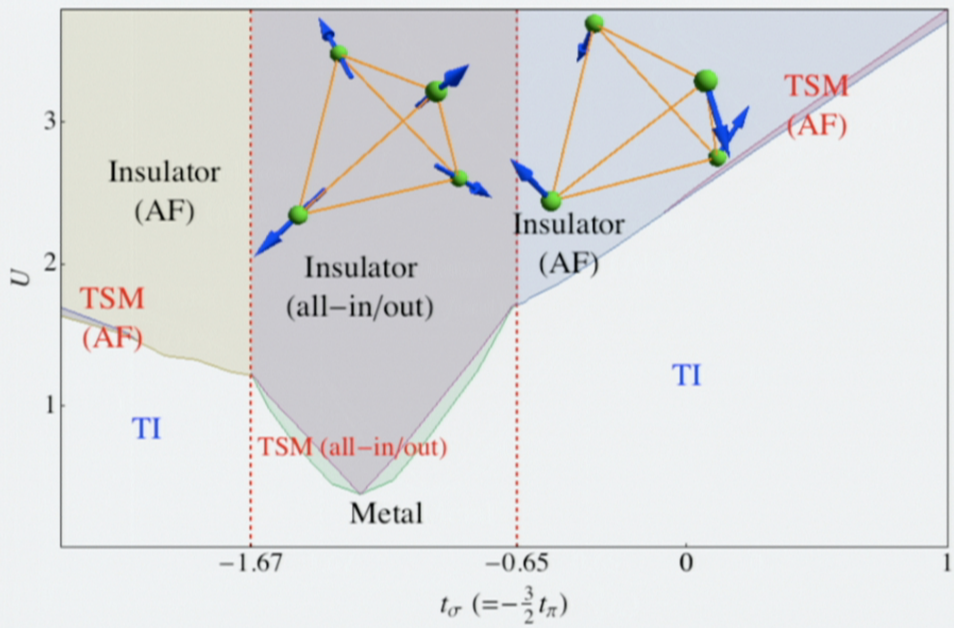


HF phase diagram

$t_{oxy} = 1$



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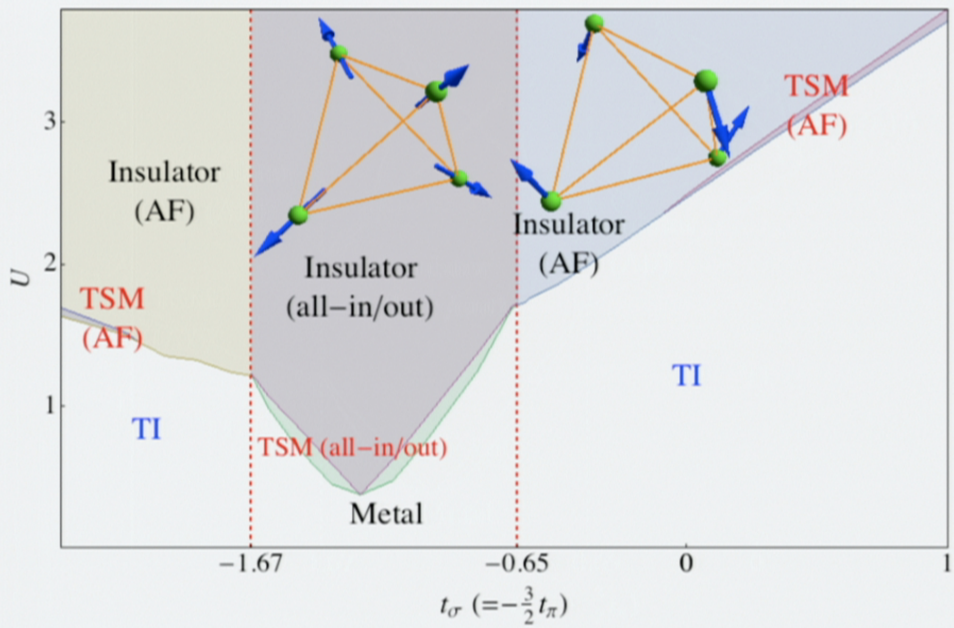
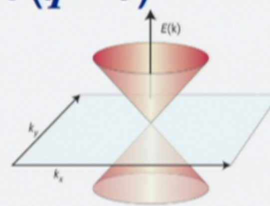


Topological Weyl semimetal

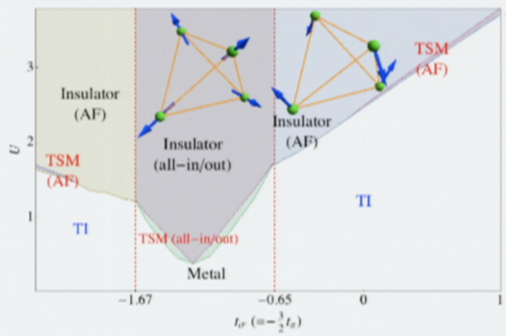
- Effective Hamiltonian near Weyl pt ($\boldsymbol{q} = 0$)

$$H = \pm v\vec{q} \cdot \vec{\sigma}$$

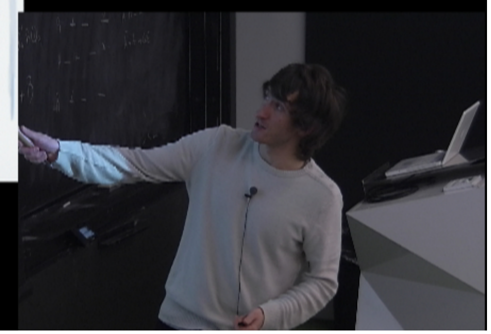


- 2-component ~ **Weyl** fermion
- Chiral (L/R handed, like massless neutrino)
  chirality = ±1
- Can't introduce mass gap
  → Topological object
- To remove, Weyl pts of opposite chirality must meet in BZ
  (need L & R Weyl fermions to make massive Dirac)

Main results



- Different MIT-s & magnetic orders
- **Weyl topological semimetal** present with different orders:
  - **All-in/out**: out of a (semi)metal (2nd order) Effects of interactions on quadratic band touching?
  - **Other chiral orders**: out of TI (1st order)



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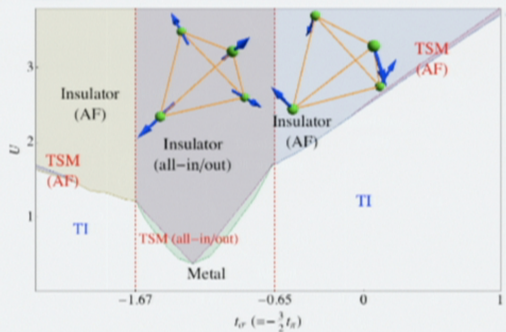

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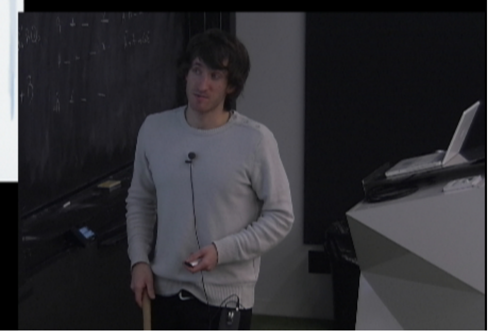
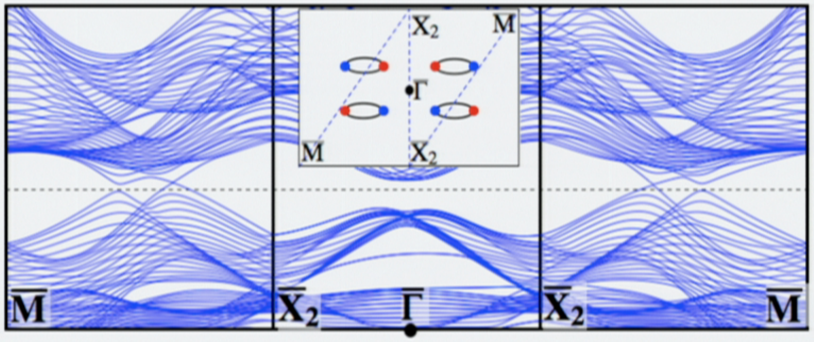


Surface States

- Fermi arcs!



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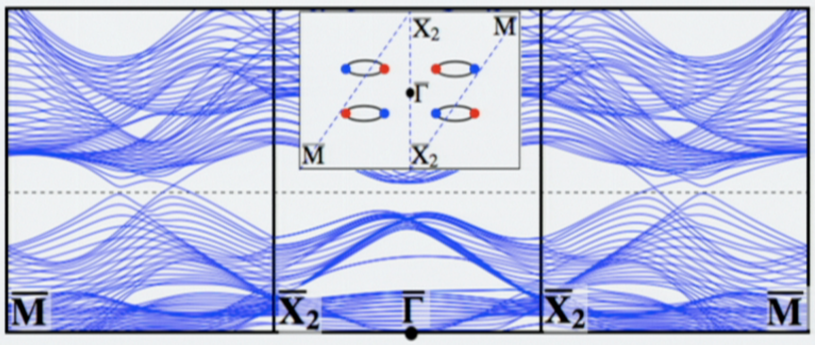
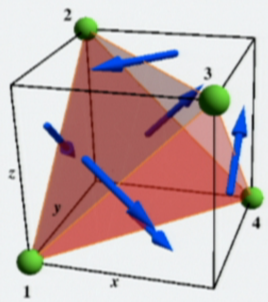


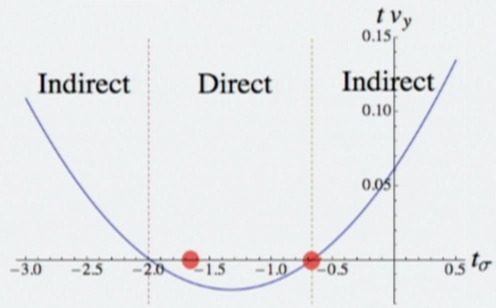
Beyond MFT: strong coupling

- U/t >> 1, get (pseudo)spin model:

$$H' = \sum_{ij} \left[J\vec{S}_i \cdot \vec{S}_j + \vec{D}_{ij} \cdot (\vec{S}_i \times \vec{S}_j) + S_i^a \Gamma_{ij}^{ab} S_j^b \right]$$

- Monte carlo + MF analysis of NN Heisenberg+DM model on pyro lattice [Elhajal et al., PRB 2005]. **Order depends on DMI**:
  - Direct: all-in/out, Indirect: continuous set





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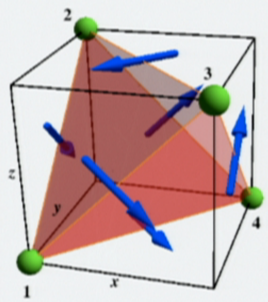

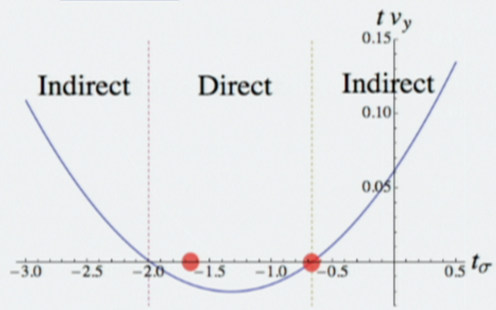

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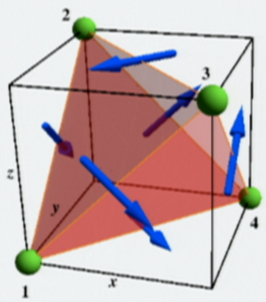
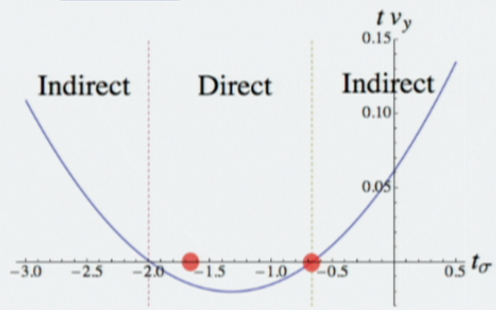
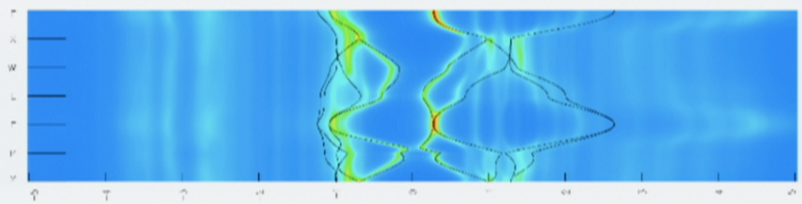




Beyond MFT: C-DMFT

[A. Go, WWK, G. S. Jeon and Y. B. Kim, in preparation.]

- Cluster = 1 u.c. = tetrahedron
- Effective bath has 8 sites
- Use Exact Diagonalization



- **Results**
  - Same magnetic order as HF
  - Stability of TI & Weyl phase with interactions
  - Studied surface states **within** DMFT: robust to correlations

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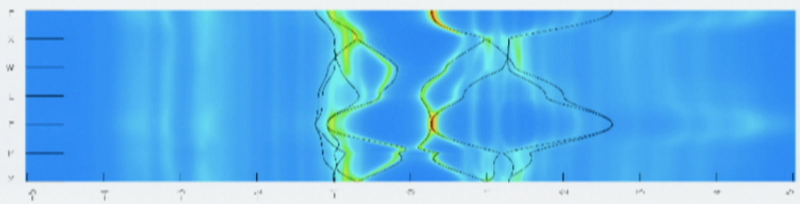

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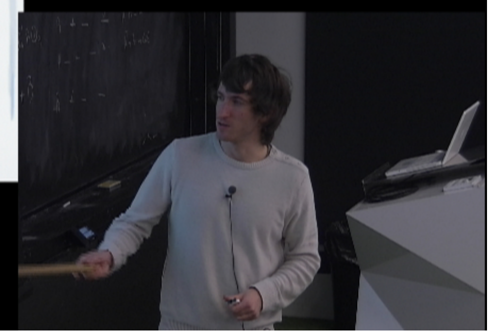


Part 2
Topological Mott insulator:
a helical spin liquid

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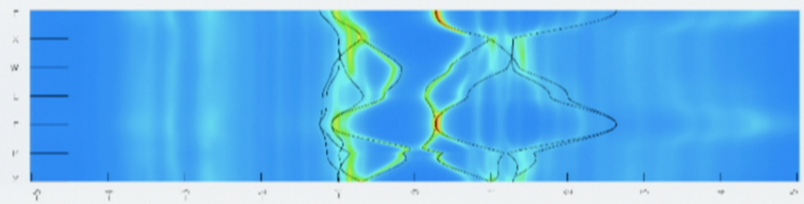

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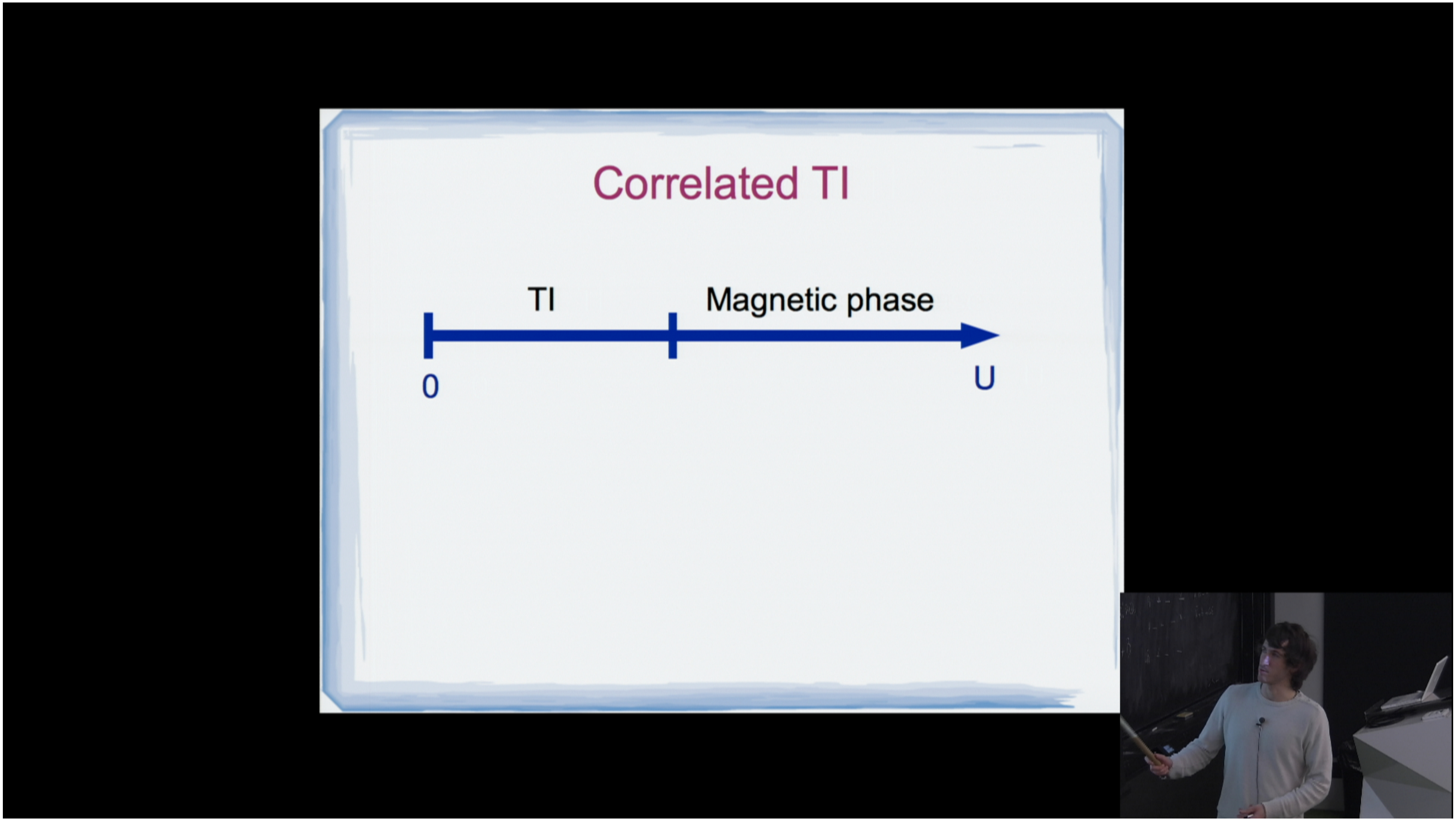
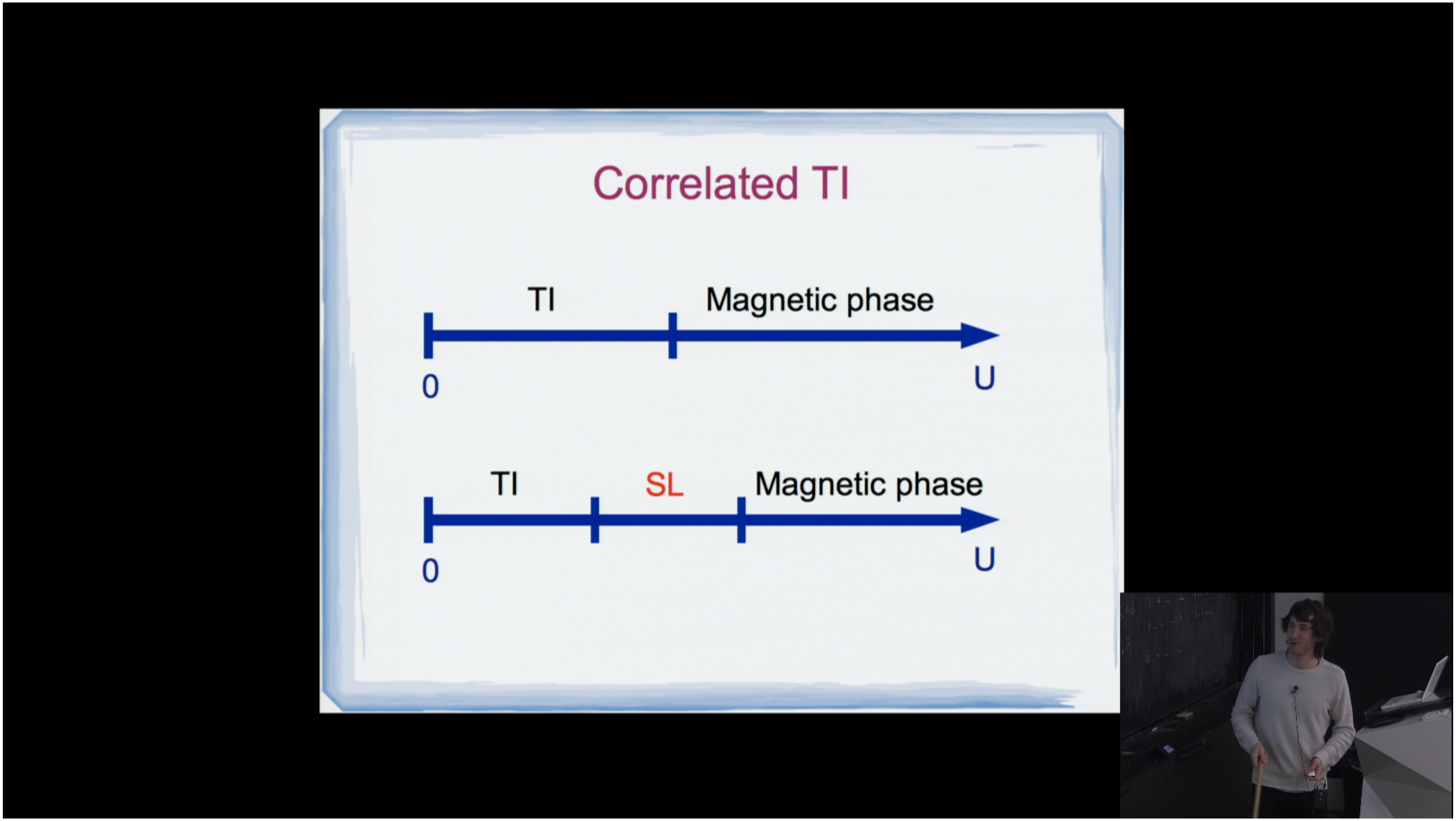

Correlated TI
TI
Magnetic phase
0
U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U
TI
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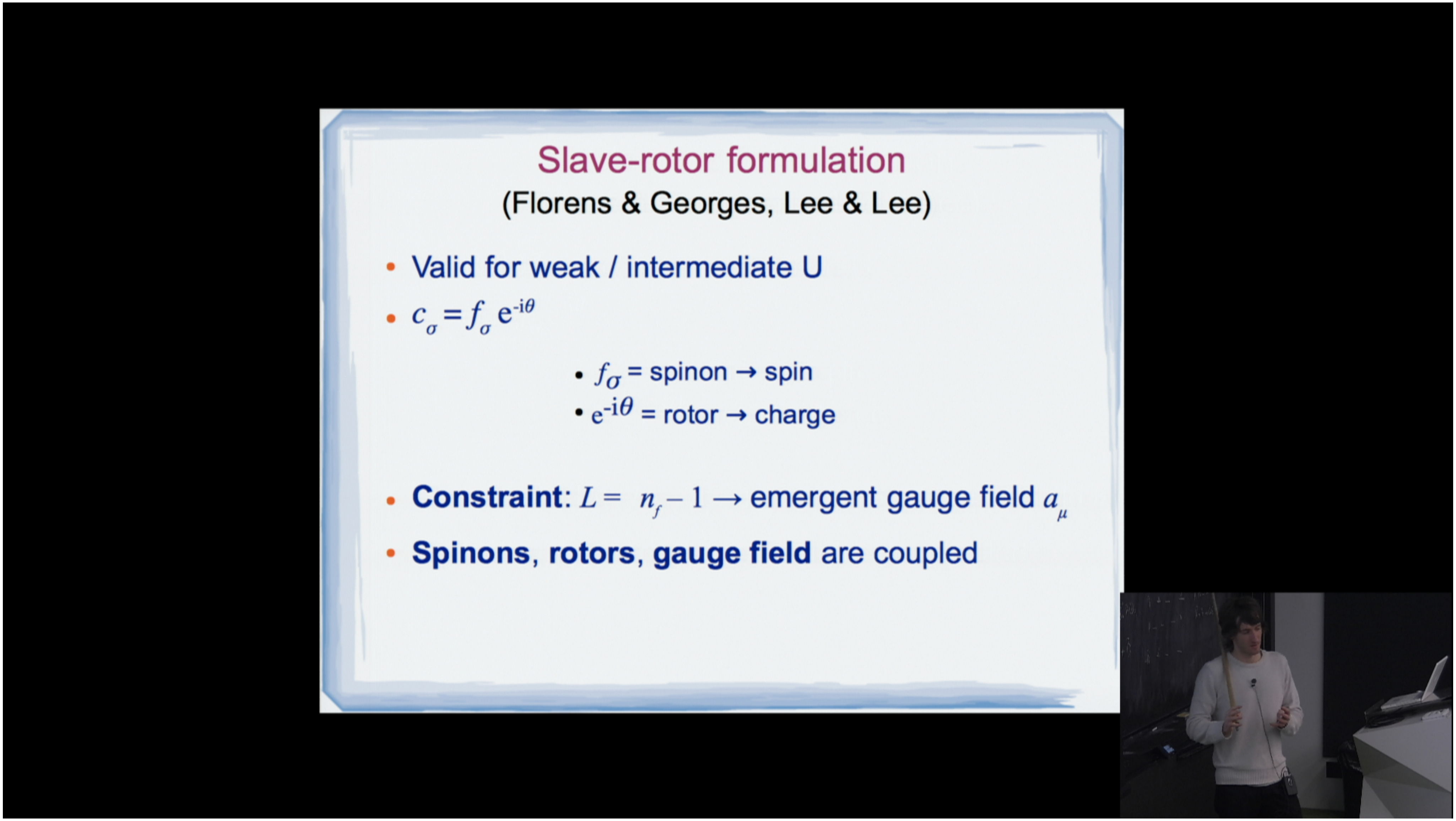
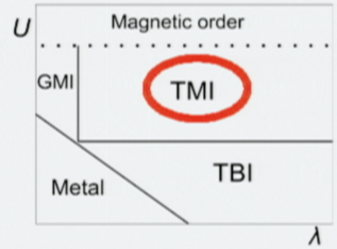
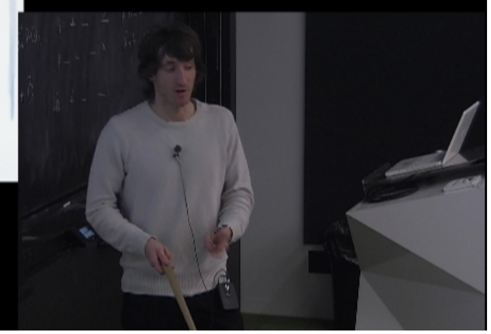

Slave-rotor formulation
(Florens & Georges, Lee & Lee)
Valid for weak / intermediate U
$c_\sigma = f_\sigma e^{-i\theta}$
f_σ = spinon → spin
$e^{-i\theta}$ = rotor → charge
Constraint: $L = n_f - 1 \rightarrow$ emergent gauge field a_μ
Spinons, rotors, gauge field are coupled

Topological Mott Insulator



- Rotors gapped
- Spinons → non-trivial U=0 band topology
- TI of spinons
  - Bulk spinons = gapped
  - Gapless spinon surface states, **helical**
- Gauge fluctuations in the **bulk**

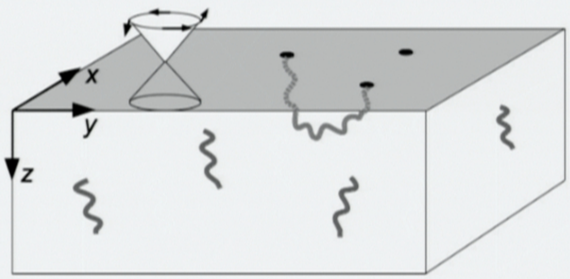


QFT: Beyond MFT

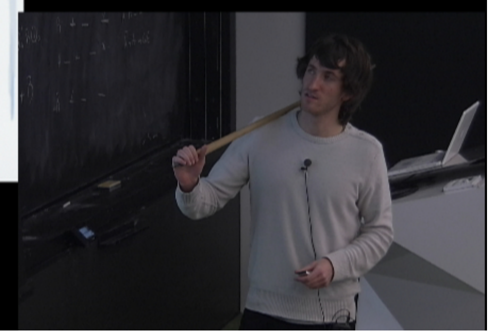
[WWK, T.P. Choy & Y.B. Kim, *PRB* (2010)]

- Dirac fermions @ finite μ:
  helical liquid of spinons
- 3D emergent gauge-b

$$f^\dagger \vec{\sigma} \cdot (\nabla - ig\vec{a}|_{z=0}) f$$



- Dirichlet BC on gauge-b → Standing waves



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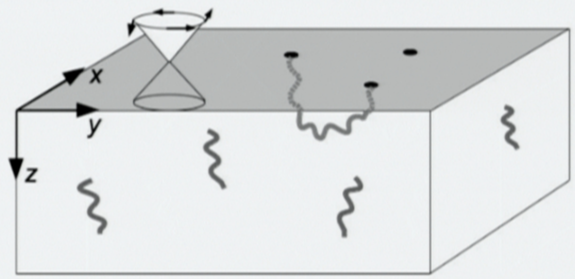

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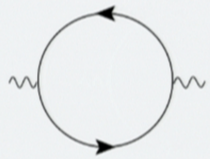
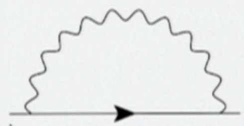
Gauge interaction as a perturbation

- *Landau damping* of gauge-b



$$\frac{|\omega|}{v_F\sqrt{q_x^2+q_y^2}}$$

- Renormalization of fermions



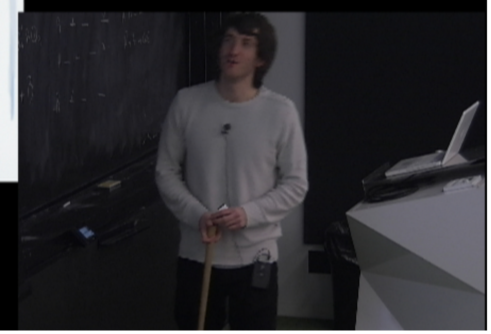
$$i\omega \ln \frac{\mu}{|\omega|}$$

Marginal

Pure 2D theory:

$$i\mathrm{sgn}(\omega)|\omega|^{2/3}$$

- RG: *g* is marginally irrelevant (caveat...)



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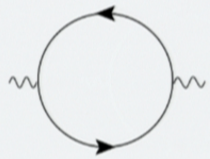

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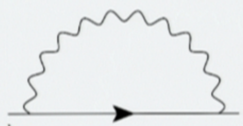

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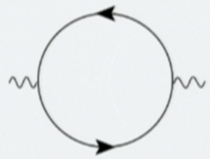

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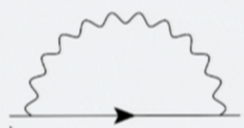

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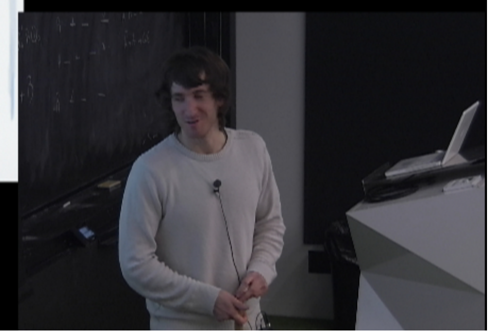
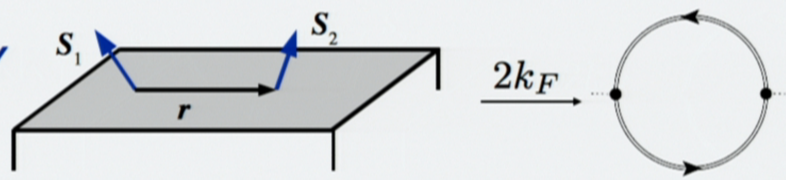
$$i\mathrm{sgn}(\omega)|\omega|^{2/3}$$

- RG: *g* is marginally irrelevant (caveat...)



Signatures of TMI

- Heat capacity: $C \propto T \ln \frac{\mu}{T}$
- RKKY

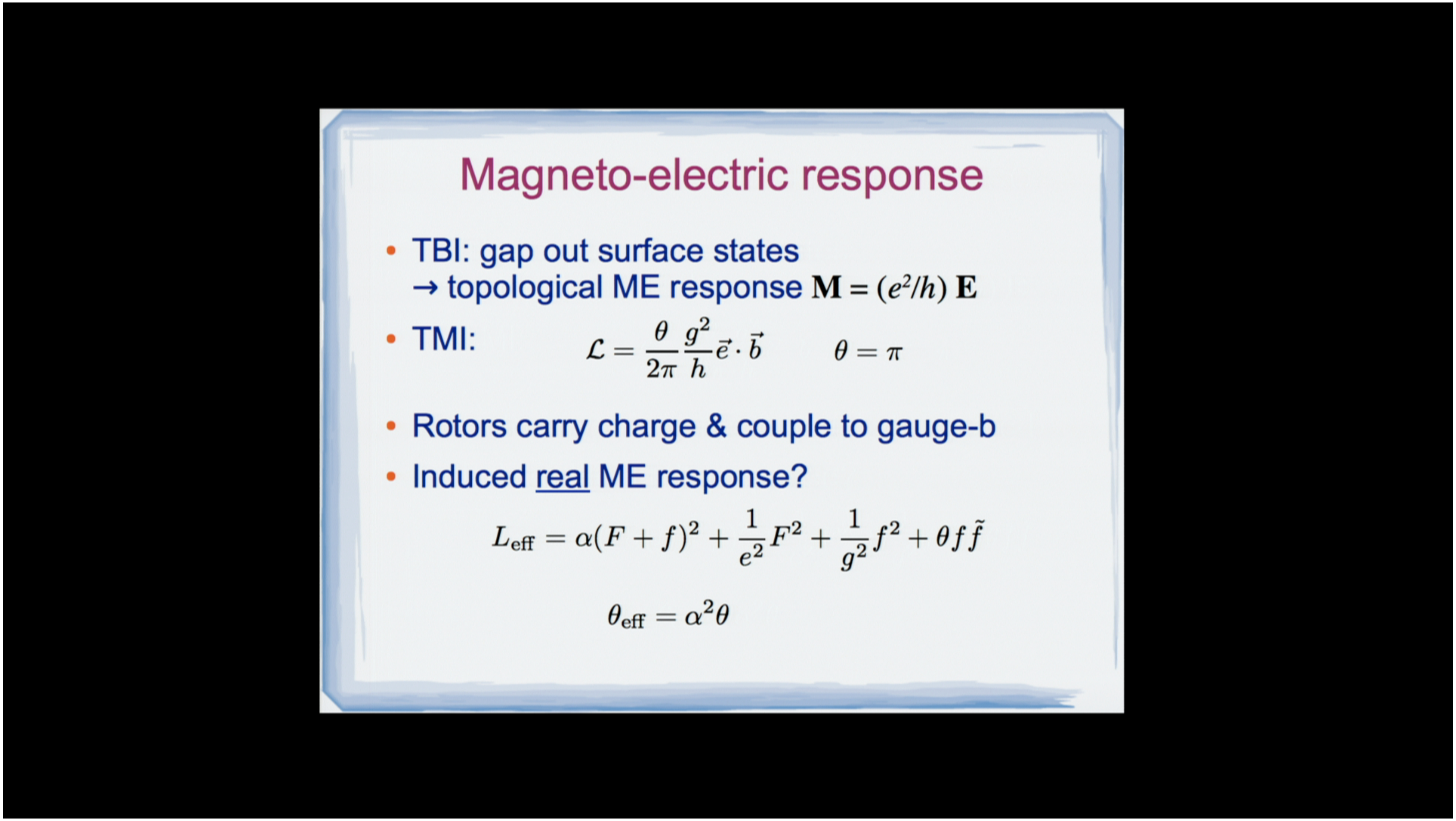


$$H_{\mathrm{RKKY}} = J_z S_1^z S_2^z + J_z(\vec{S}_1 \cdot \hat{r})(\vec{S}_1 \cdot \hat{r}) + J_{\mathrm{DM}}\, \hat{r} \cdot (\vec{S}_1 \times \vec{S}_2)$$

$$J_i(r) \propto \frac{1}{r^2 \ln(k_F r)}$$

TMI vs TI

	TMI	TI
C	$T \ln T$	T
RKKY	$1/(r^2 \ln k_F r)$	$1/r^2$
Charge resp.	no	surface
Thermal resp.	yes	yes
Magnetoelectric	?	$\theta = \pi$


Magneto-electric response
TBI: gap out surface states
→ topological ME response $\mathbf{M} = (e^2/h)\,\mathbf{E}$
TMI: $\mathcal{L} = \frac{\theta}{2\pi}\frac{g^2}{h}\vec{e}\cdot\vec{b}$ $\theta = \pi$
Rotors carry charge & couple to gauge-b
Induced real ME response?
$L_{\text{eff}} = \alpha(F+f)^2 + \frac{1}{e^2}F^2 + \frac{1}{g^2}f^2 + \theta f\tilde{f}$
$\theta_{\text{eff}} = \alpha^2\theta$

Magneto-electric response

- TBI: gap out surface states
  → topological ME response $\mathbf{M} = (e^2/h)\,\mathbf{E}$
- TMI: $\mathcal{L} = \frac{\theta}{2\pi}\frac{g^2}{h}\vec{e}\cdot\vec{b} \qquad \theta = \pi$
- Rotors carry charge & couple to gauge-b
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$$L_{\text{eff}} = \alpha(F+f)^2 + \frac{1}{e^2}F^2 + \frac{1}{g^2}f^2 + \theta f\tilde{f}$$

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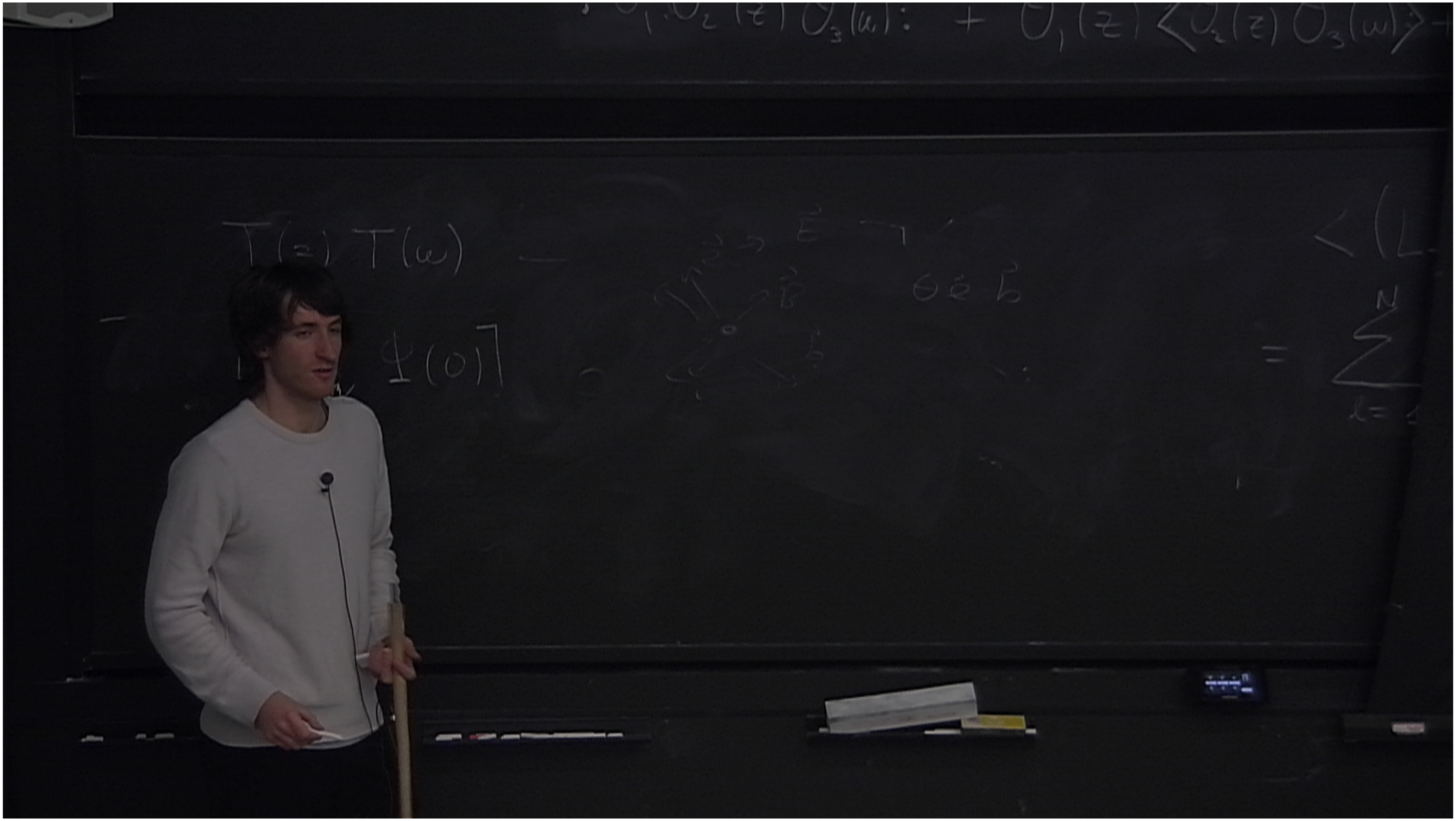

T(z) T(w)

Dyons?

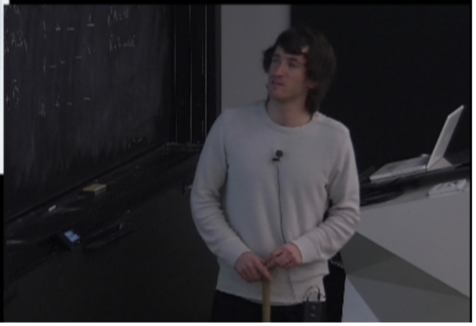
- Emergent gauge field is compact (lattice) → magnetic monopoles
- Θ-term → MM carry half-integer gauge *electric* charge → dyon [Witten, Rosenberg & Franz]

$$\mathcal{L} = \frac{\theta}{2\pi}\frac{g^2}{h}\vec{e}\cdot\vec{b}$$

- Condensation dyons → confined "conventional" phase

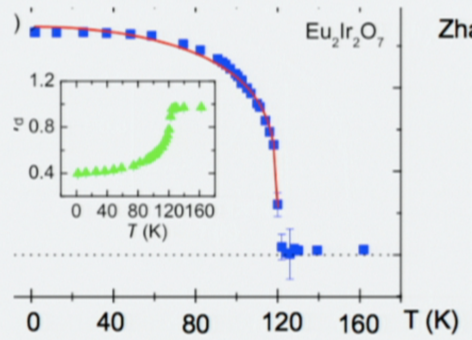
Conclusions

- Part 1: Microscopic Hamiltonian for the pyro iridates
  - Captures TI, Weyl semimetal, mag orders
  - Robustness of TI & Weyl phase with correlations
- Part 2: Topological Mott Insulator
  - Novel SL: charge-stripped TI
  - Emergent gauge field is renormalizes observables
  - Tunable magnetoelectric effect, dyons?



Experiments: Magnetism II

- muSR: sharp precession frequency below T_{MIT} = 120 K



Zhao et al., PRB (2011)

Experiment: Magnetism I

- No hysteresis: no net mag moment
- Magnetic susceptibility Feature @ ~150 K => mag transition
- Spin glass?
- Arises from Ir sites (Y not mag)

$Y_2Ir_2O_7$