Strong correlation effects in topological quantum phase transitions

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...when Correlation meets Topology

Correlated crew...

G.Sangiovanni

M.Capone

Topological crew...

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erc

DEMOCRITOS
DEmocritos MOdeling Center for Research In aTOmistic Simulation
IOM

ma per seguir virtute e canoscenza
SISSA

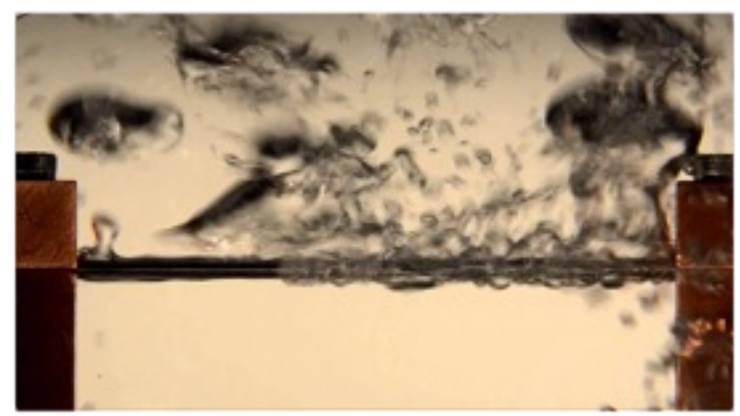
Introduction.

The phases of the matter are usually classified according to Ginzburg-Landau (*symmetry breaking*) theory…

Magnetism

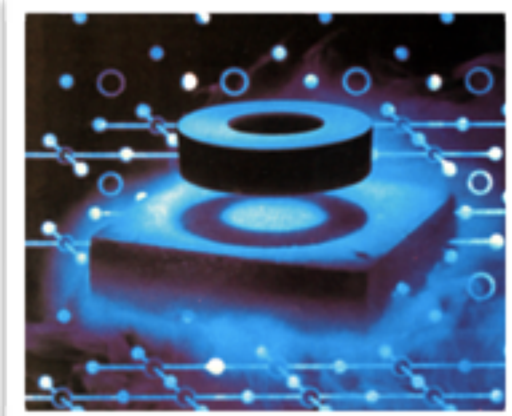
magnetization M

Liquid-gas



density difference n(L)-n(G)

"Superconductivity"



pair amplitude ψ

local order parameter

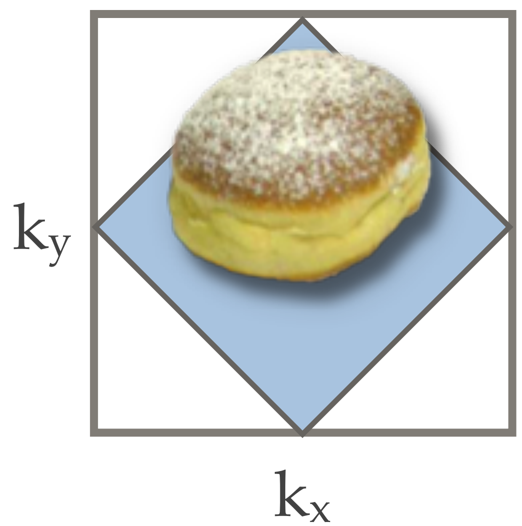
Experimental detectability!

Introduction.

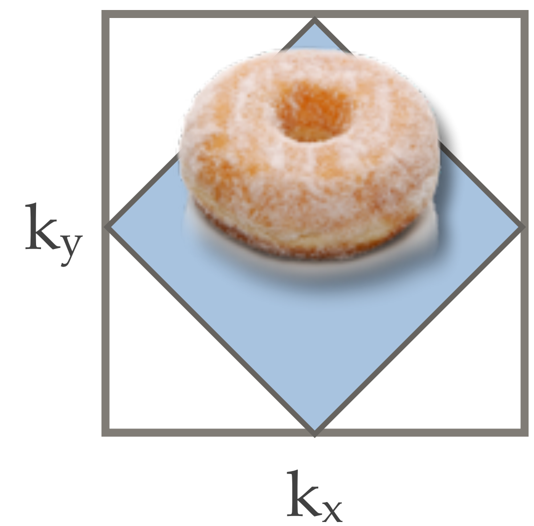
Last years witnessed the emergence of the concept of

TOPOLOGICAL INSULATORS

quantum materials which elude the conventional G-L paradigm…



Vs.



global topological invariant

hard to relate with the bulk observables

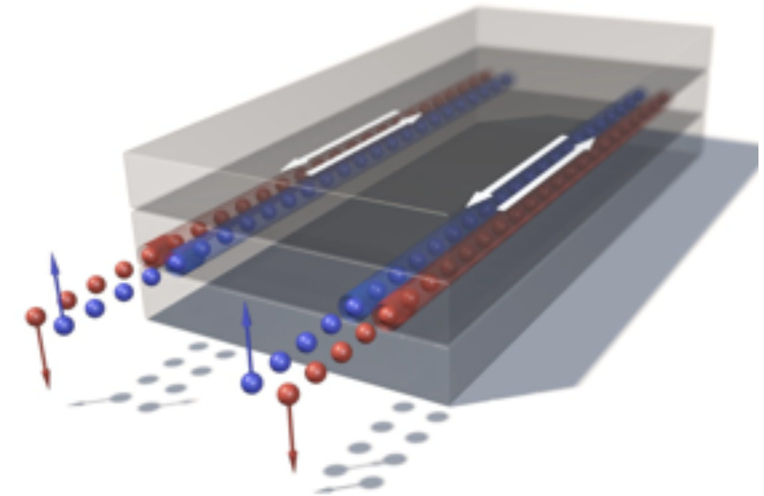
TI + geometric detour

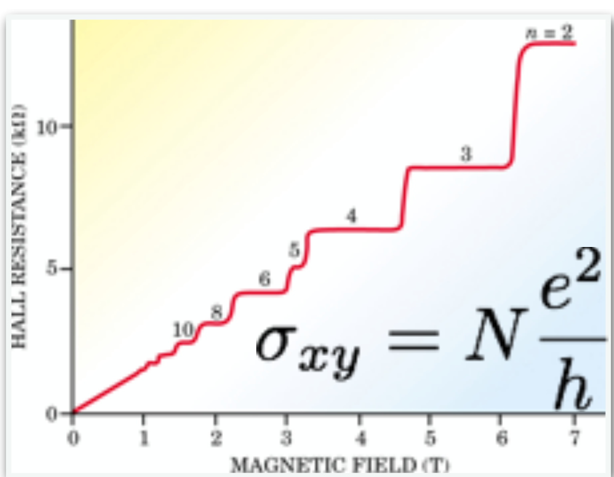
what is a TI?

a bulk (band) insulator + with *gapless* edge modes.

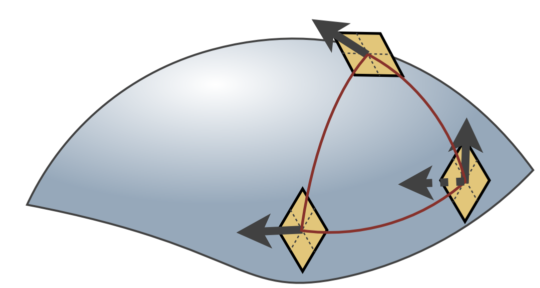
Dirac semi-metal + *Spin-Orbit Coupling*

(Haldane PRL88, Kane,Mele PRL05)





States classified in terms of the *Topological Properties* of the Hilbert space of Bloch functions*:*



Berry connection: $\mathcal{A}_n = \langle u_n(k)| - i\nabla_k |u_n(k)\rangle$ *parallel transport of Block states*

Berry curvature: $\mathcal{F}_n = \nabla_k \times \mathcal{A}_n$ *Gauss-Bonnet:* $N_n = \frac{1}{2\pi}\int_{BZ} d^2k\mathcal{F}_n$

N is the **Chern number** —> Hall cond., # edge states, Z_2 invariant

BHZ model *(quantum spin Hall insulator)*

Initial focus on graphene but small SOC (*gap ~ 10^{-3}meV*)

(Kane,Mele PRL 2005)

Idea: look for systems with a larger SOC.

(Bernevig et al Science 2006)
(Konig et al Science 2007)

BHZ model:

2 QHI + Time Reversal Symmetry.

$$H = \begin{pmatrix} \mathbf{h}(\mathbf{k})\uparrow & \mathbf{0} \\ \mathbf{0} & \mathbf{h}^*(-\mathbf{k})\downarrow \end{pmatrix}$$

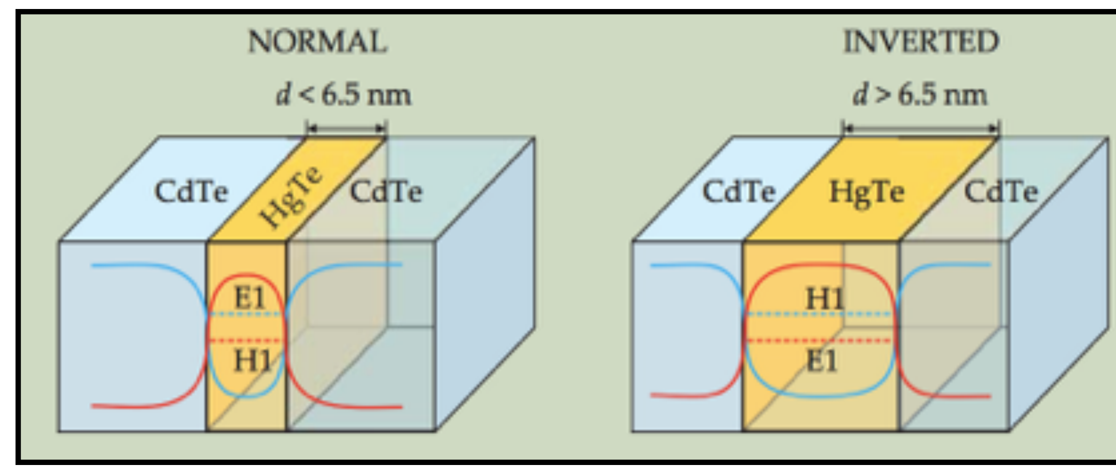
Spin structure

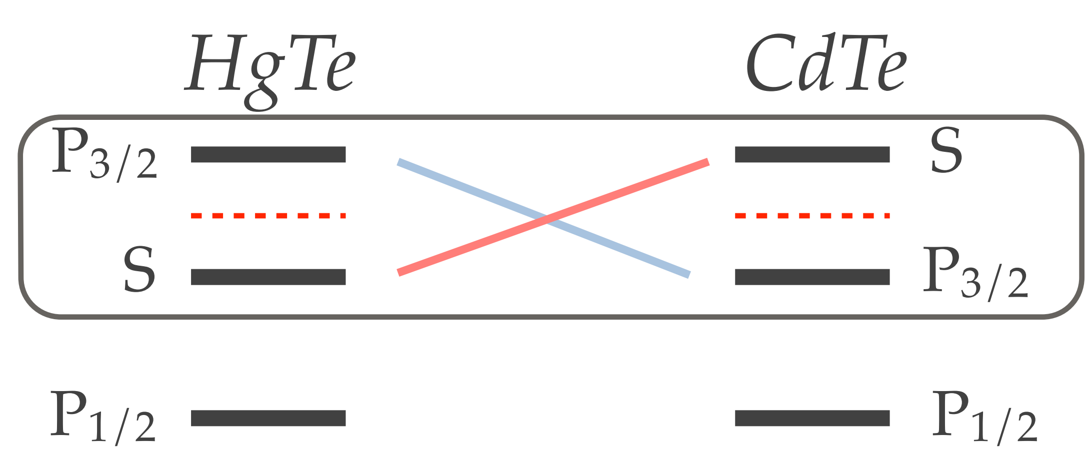
$$\mathbf{h}(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \tau$$

Orbital pseudo-spin structure

$$\mathbf{d}(\mathbf{k}) = \begin{pmatrix} \lambda \sin k_x \\ \lambda \sin k_y \\ M - \cos k_x - \cos k_y \end{pmatrix}$$

CdTe/HgTe quantum wells.

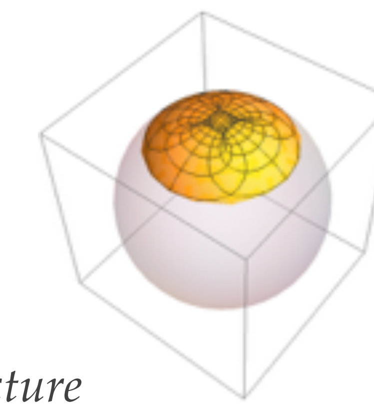




Topological QPT

$\mathcal{C}_1$=0

BHZ description of topological transition:



spin texture

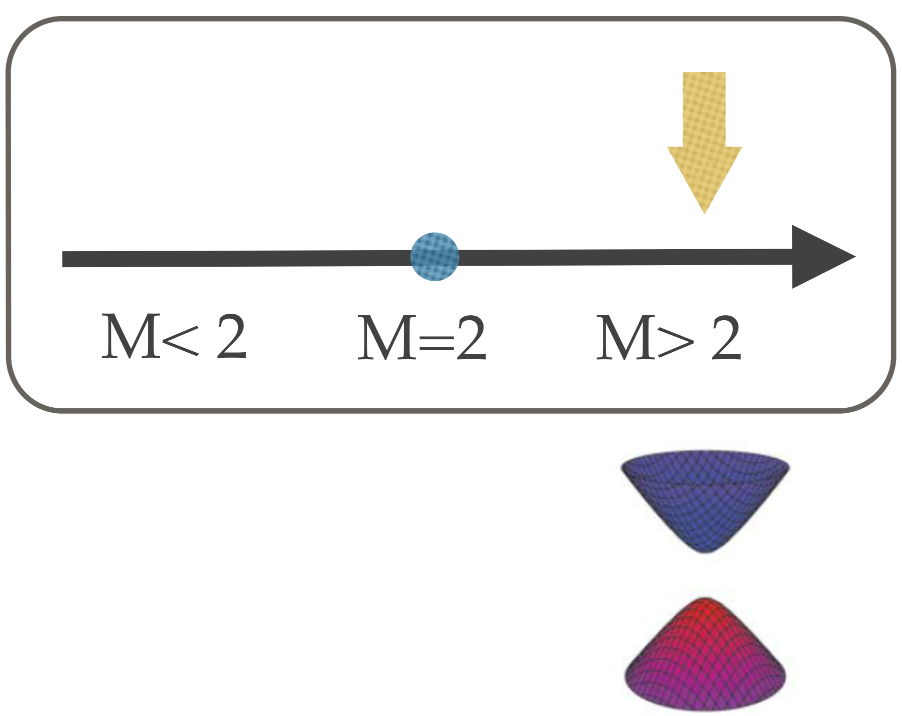
M> 2

$$\mathbf{h}(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \tau$$

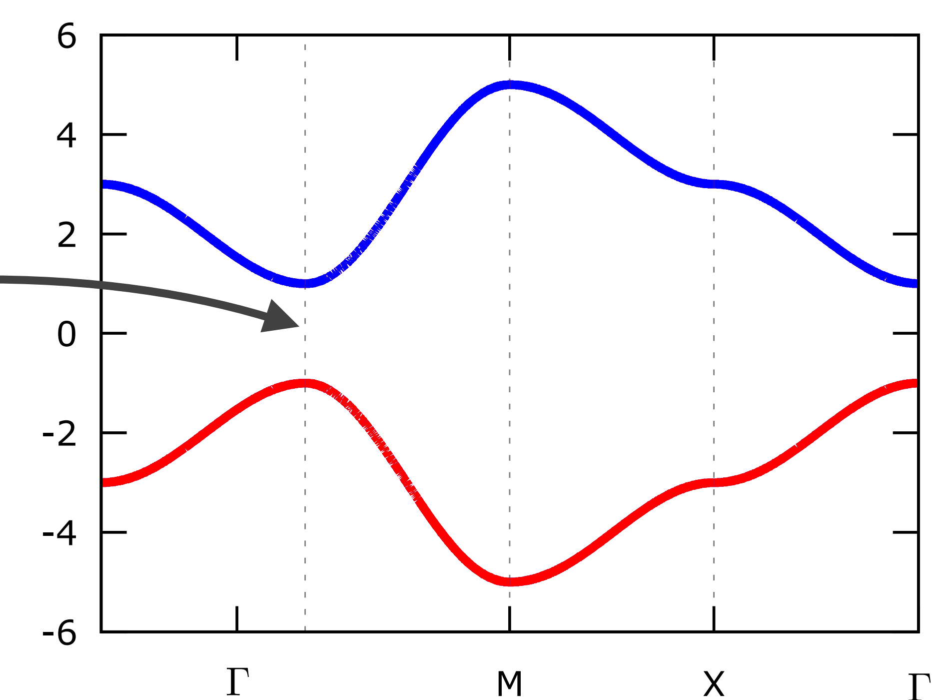
$\mathbf{d}(\mathbf{k})$

Continuous Topological Quantum Phase Transition

band structure evolves smoothly with control parameters…



trivial band insulator



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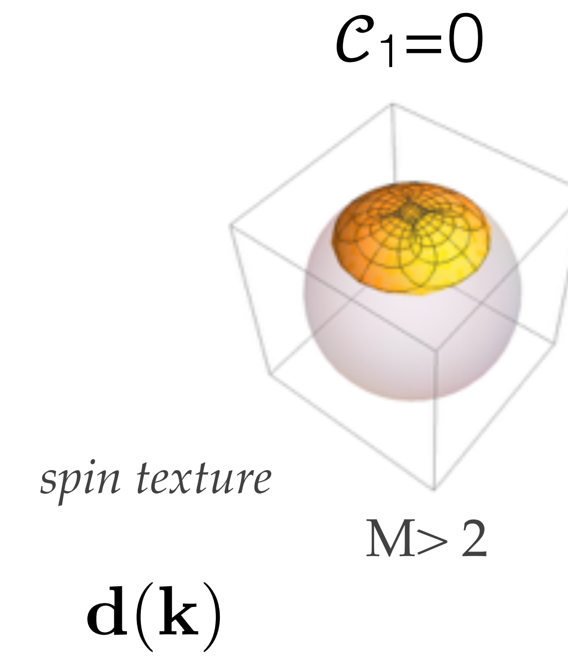

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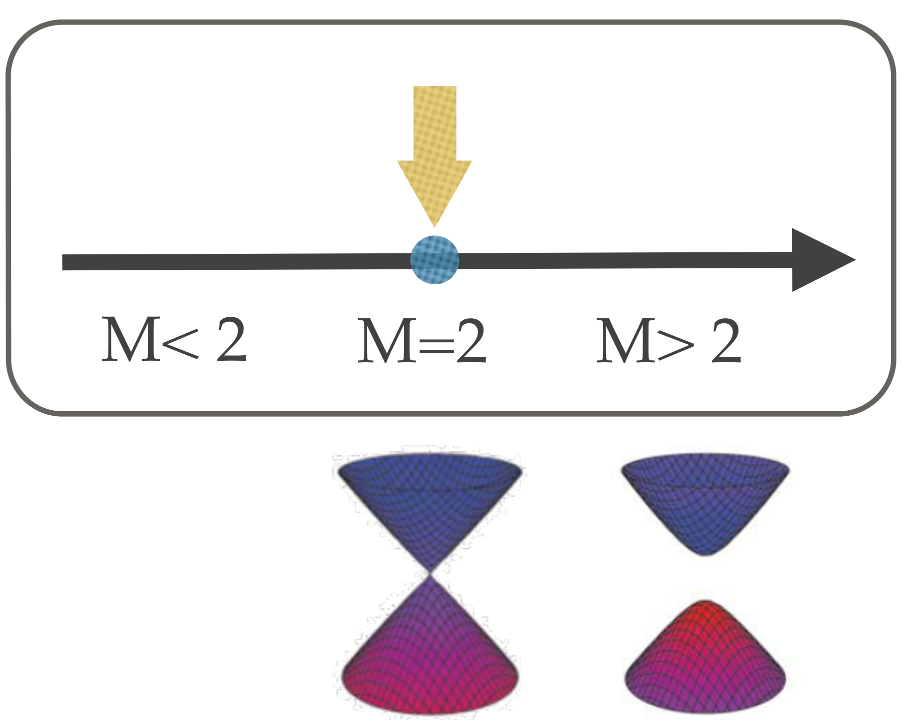

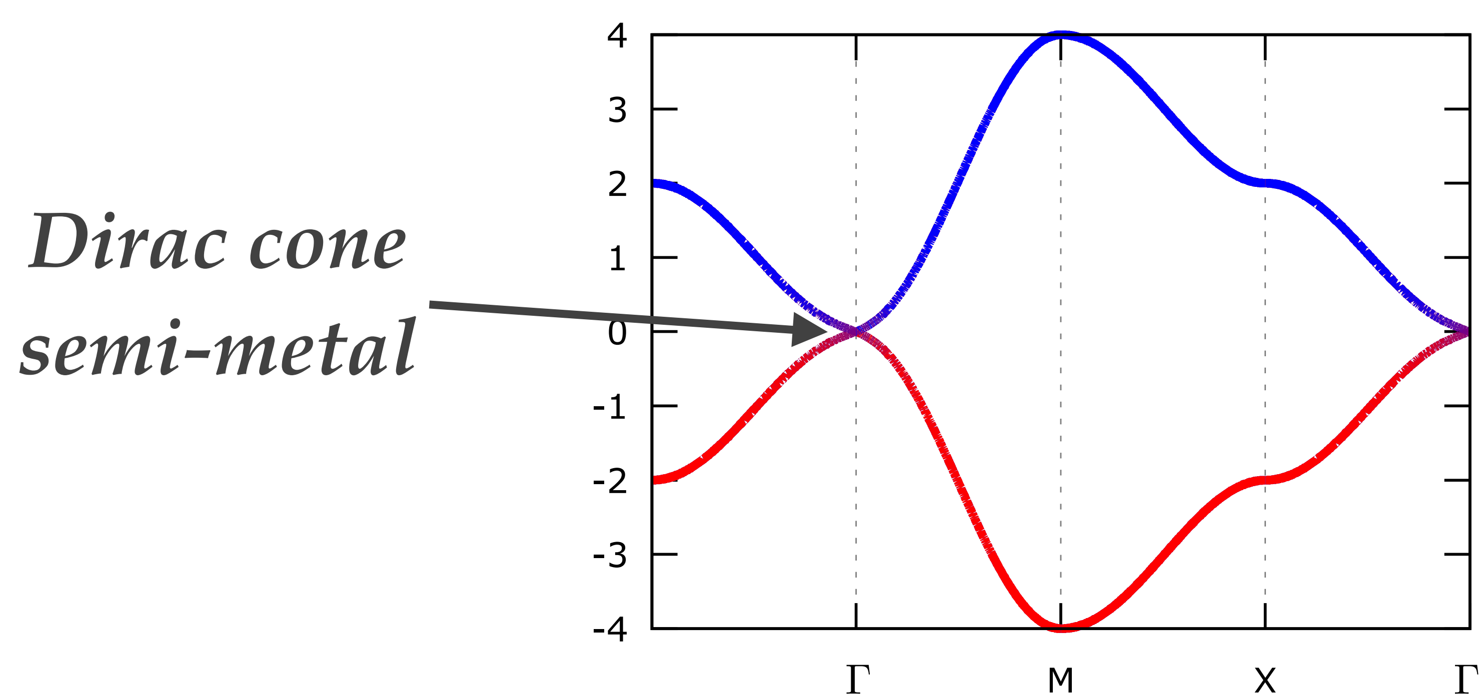

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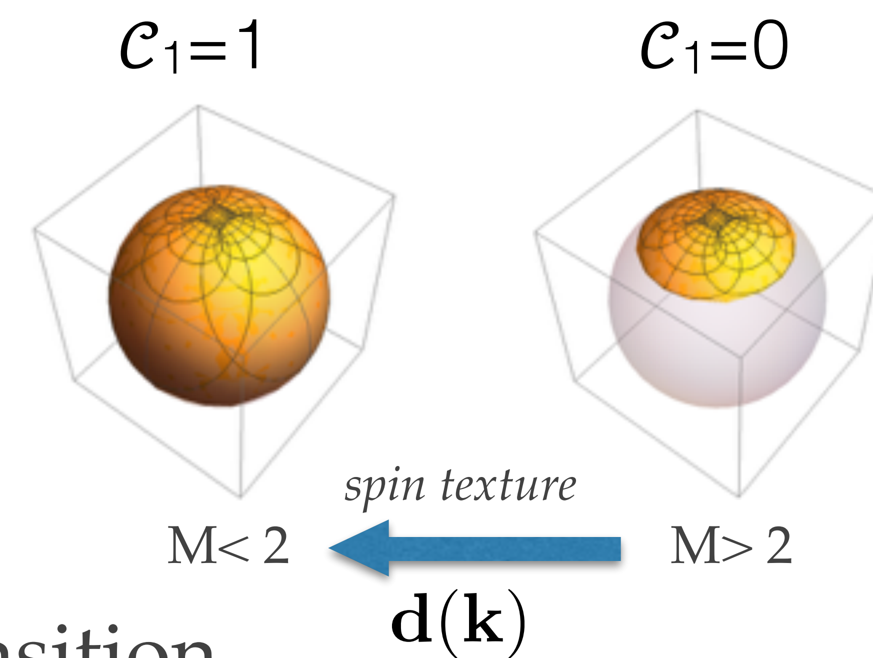

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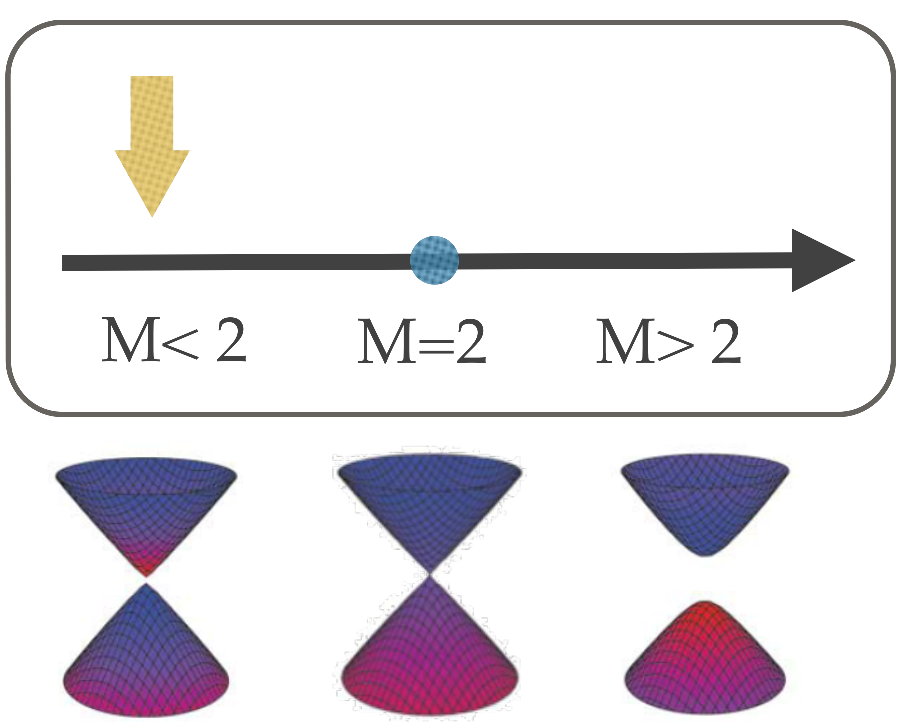
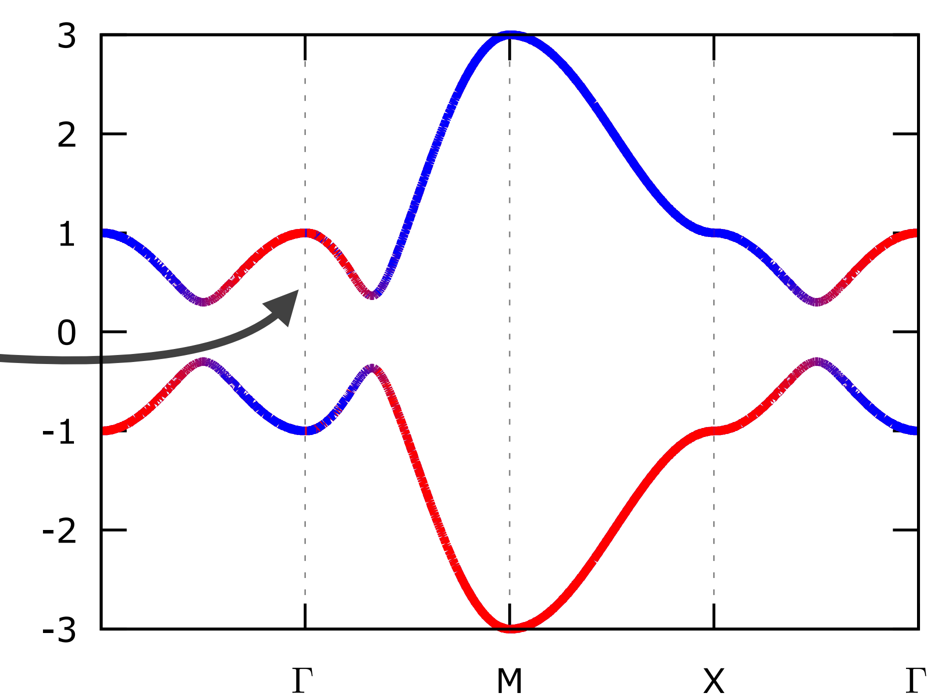
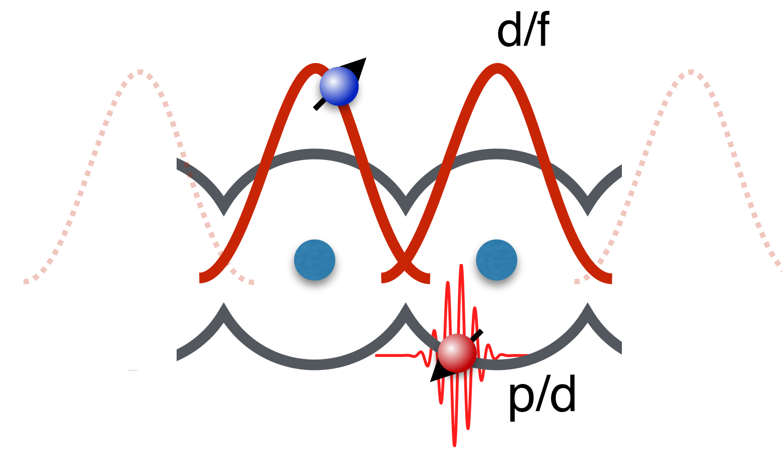


band inversion
QSH insulator



Interaction + SOC

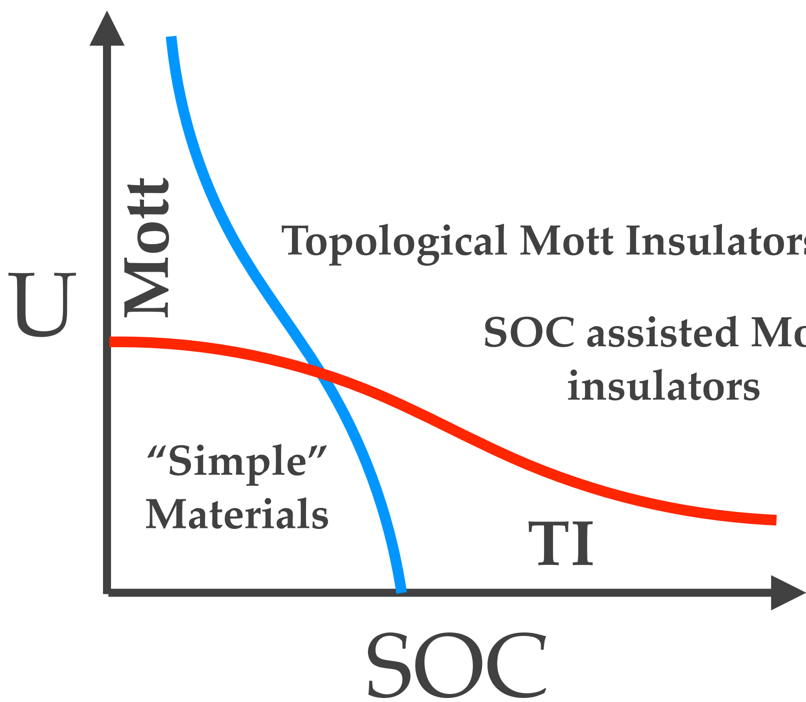


Quest for larger SOC…

…heavy elements compounds (*5d/4f*)…

*e.g. hexaborides **Sm/Pu**B_6,* Dzero et al. PRL 2010

*Ir-based pyrochlores: e.g. Sr_2**Ir**$_2O_7$, etc..* D. Pesin, L. Balents, NP 2010



from L.Balents website

…large electronic interaction,

SOC strongly reacts to it

Hohenadler , Assad. Journal of Phys. 2013

What is the fate of the TQPT?

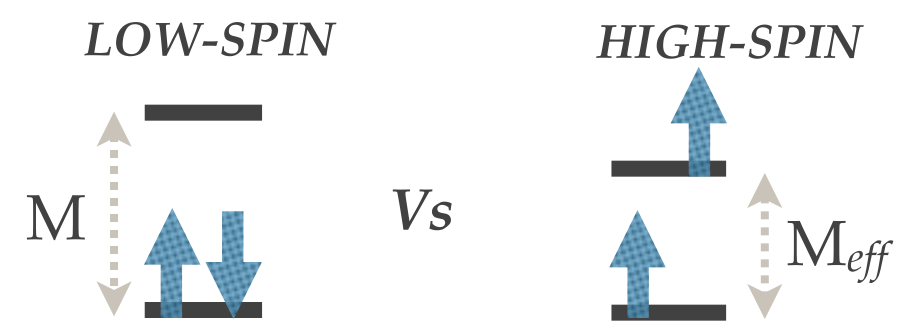
BHZ + Hubbard

Let's take into account multi-orbital **interactions**:

$$H = \begin{pmatrix} \mathbf{h}(\mathbf{k}) & \mathbf{0} \\ \mathbf{0} & \mathbf{h}^*(-\mathbf{k}) \end{pmatrix} + (U-J)\underbrace{\frac{N_{\rm i}(N_{\rm i}-1)}{2}}_{} - J\left(\overset{density}{\frac{N_{\rm i}^2}{4}} + \overset{spin}{S_{z{\rm i}}^2} - \overset{orbital}{2T_{z{\rm i}}^2}\right)$$

Hund's coupling: *maximize* $\langle S^2{}_z \rangle$

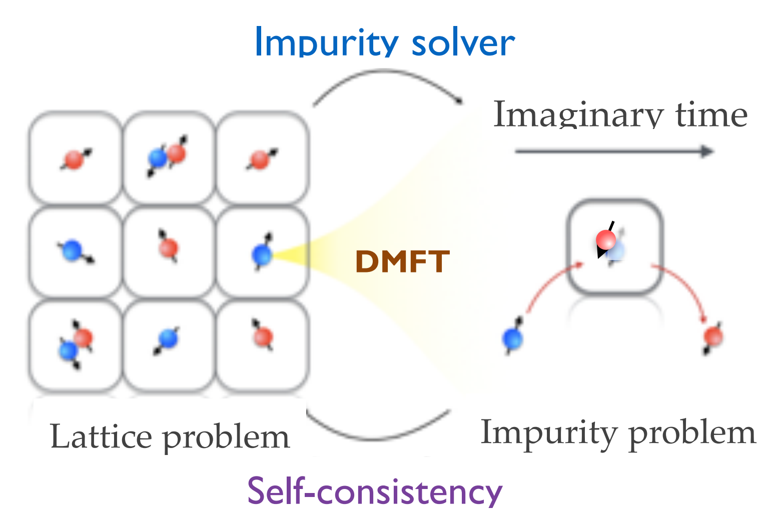
minimize $\langle T^2{}_z \rangle$



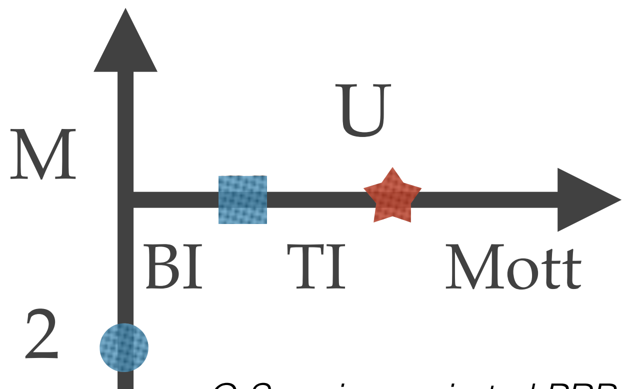
Dynamical Mean-Field Theory at T=0.

Dynamical effects of interaction are encoded in the self-energy function.

$$\hat{\Sigma}(\omega) = \mathrm{Re}\Sigma(\omega)\sigma_0 \otimes \tau_z + \mathrm{Im}\Sigma(\omega)\sigma_0 \otimes \tau_0$$



Interaction driven transitions



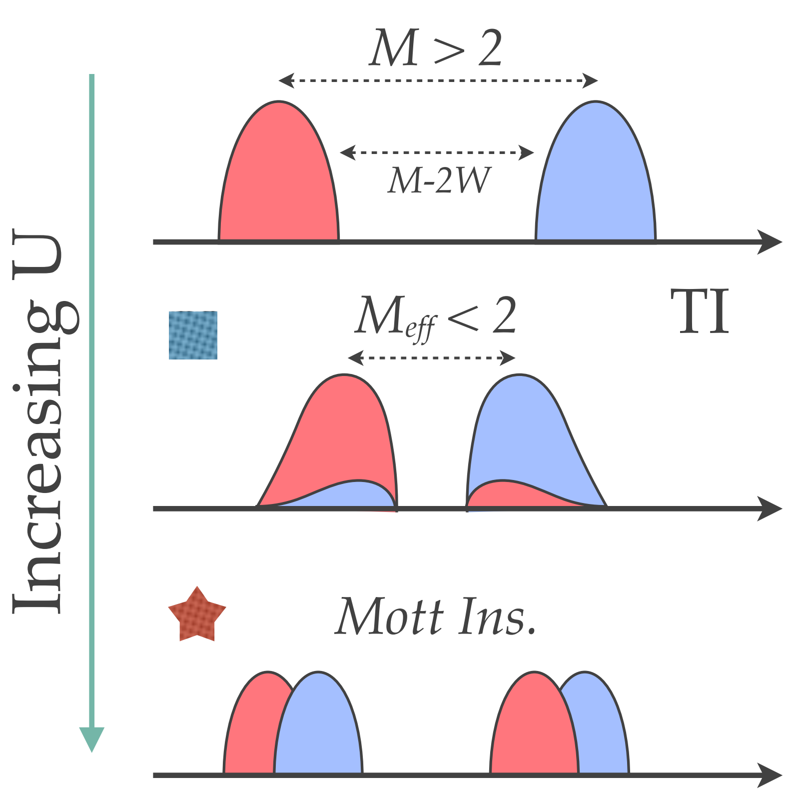
G.Sangiovanni et al PRB 2012

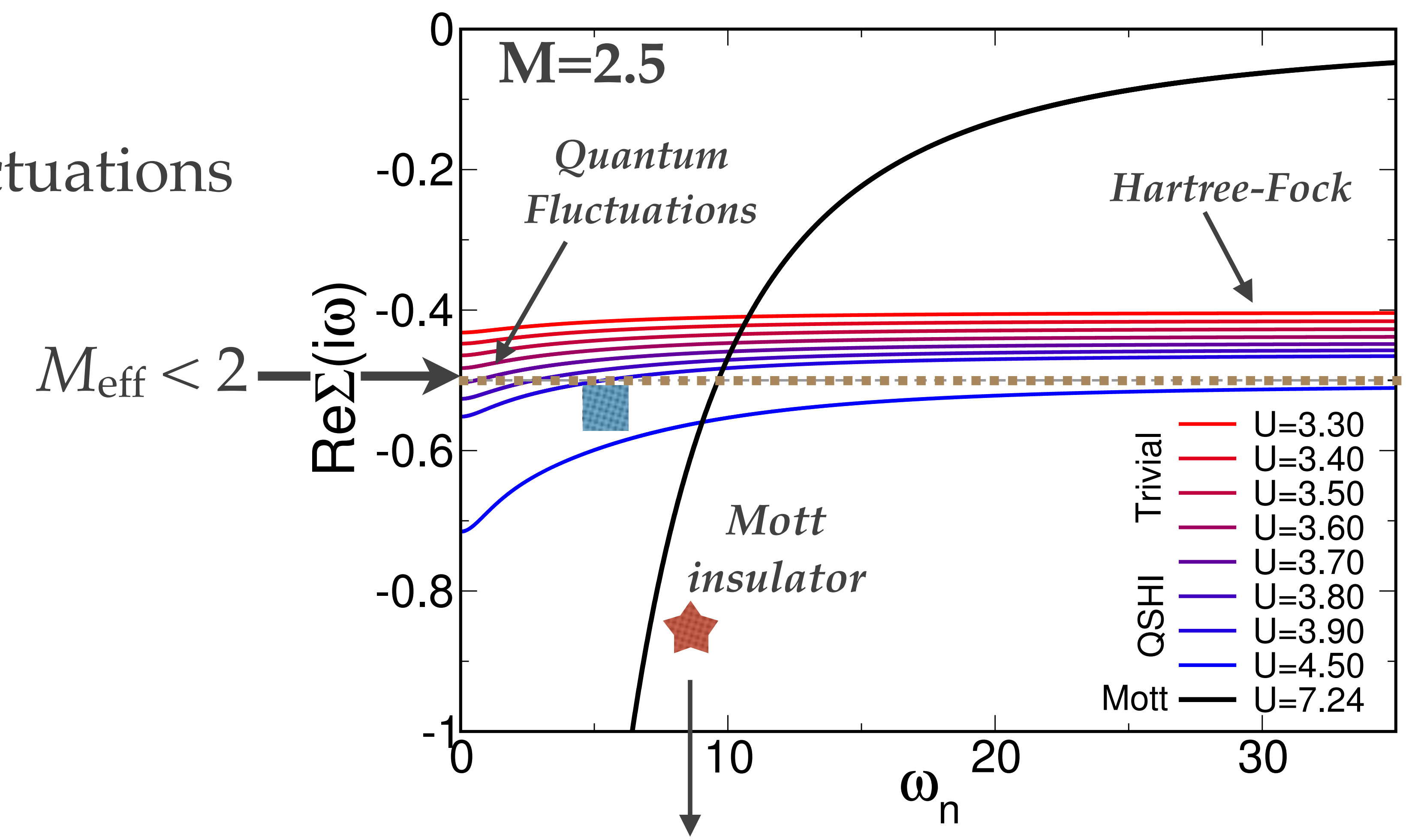
***AA** et al PRL 2015*

- Effective reduction of Mass term

$$M_{\text{eff}} = M + \text{Tr}[\tau_z \hat{\Sigma}(0)]/2$$

- (Interaction) Quantum Fluctuations driven **TQPT**





- Increasing U drives the system into a **Mott phase** with one electrons per orbital.

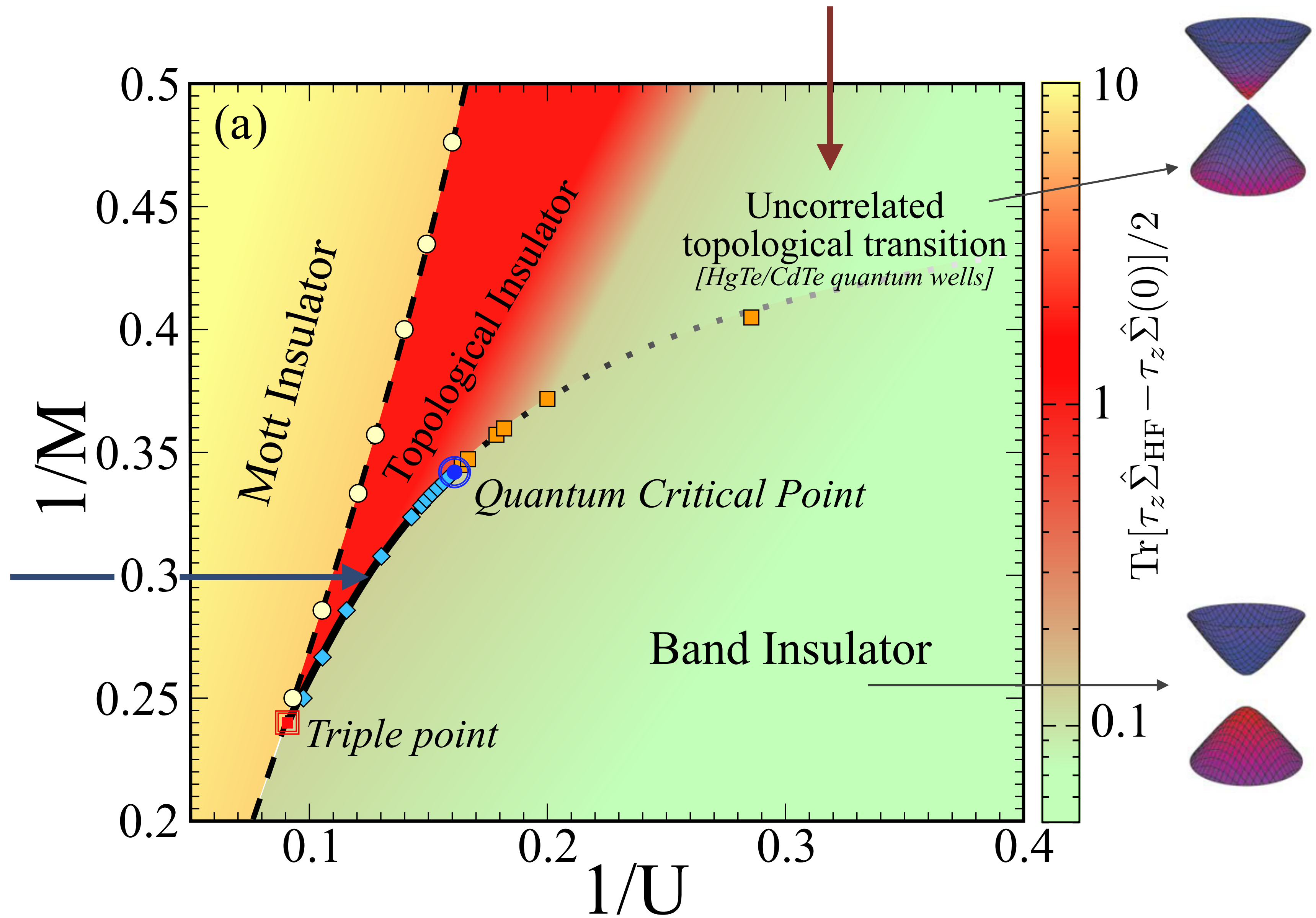
Phase-diagram

Phase diagram (*flipped view*): 1/M vs. 1/U. ***Liquid-Gas analogy***.

Color code reflects correlation degree: $\mathrm{Tr}[\tau_z \hat{\Sigma}_{\mathrm{HF}} - \tau_z \hat{\Sigma}(0)]/2$

Weak coupling: Hartree-Fock like. Continuous as the U=0 case.

Strong coupling:
1st order transition!
many-body character
strongly correlated
different ground states



AA *et al PRL 2015*

recently re-discovered in
Rau, Goswami et al arXiv: 1507.00722

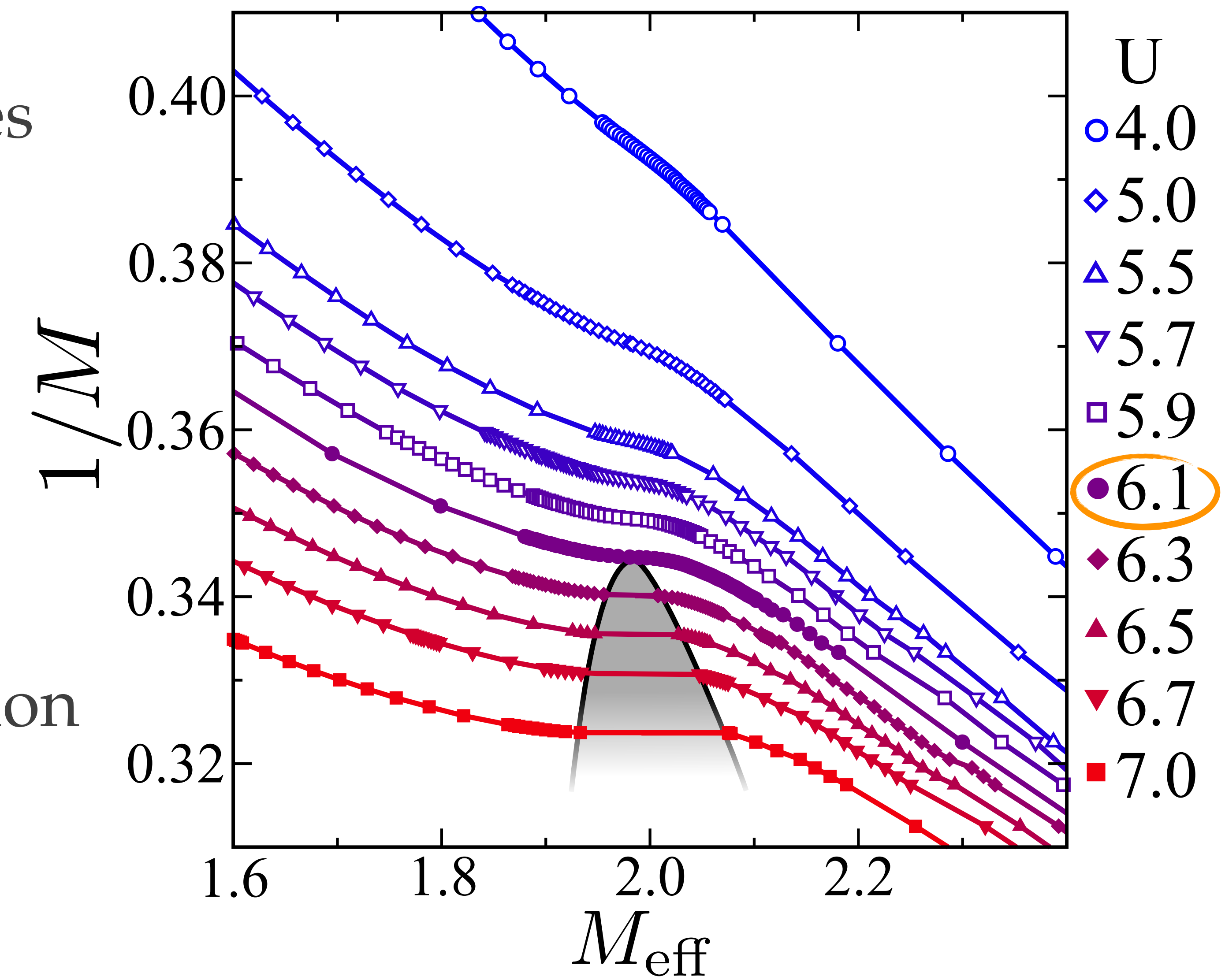
Topological QPT

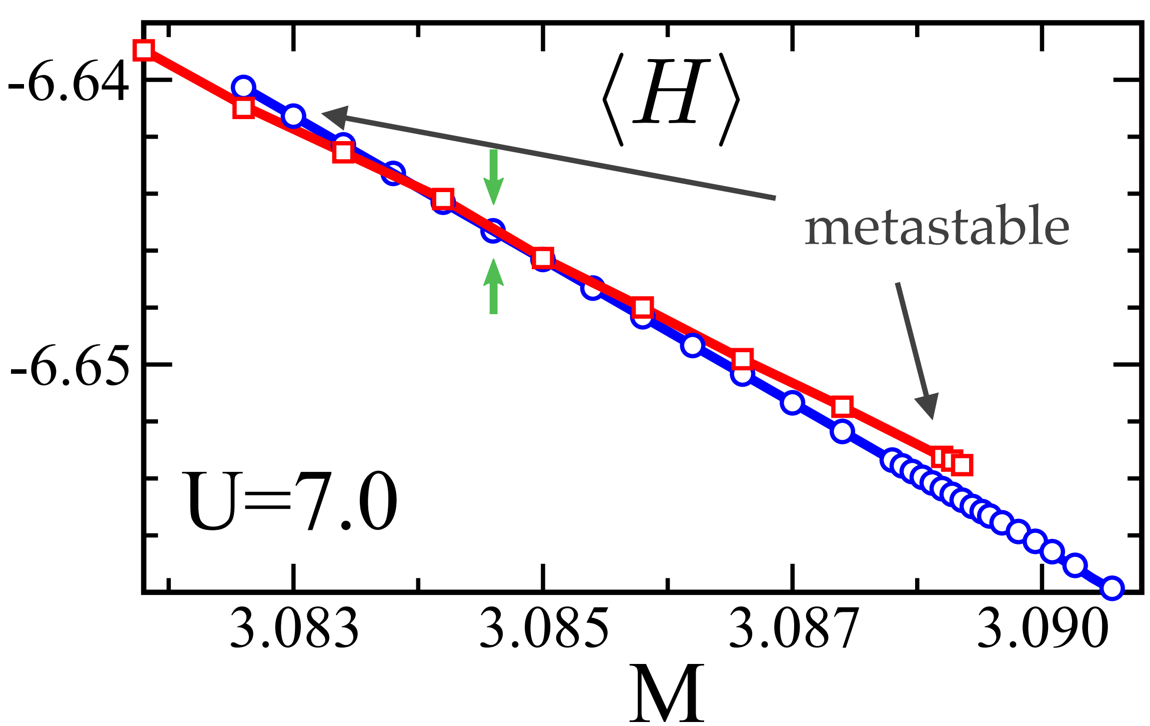
A clear picture from the *iso*-U curves

- For U<U_c continuous transition
- For U=U_c critical behavior
- For U>U_c discontinuous transition

$$\Delta M_{\rm eff} = M_{\rm eff}(BI) - M_{\rm eff}(QSH)$$

is the order parameter of the transition

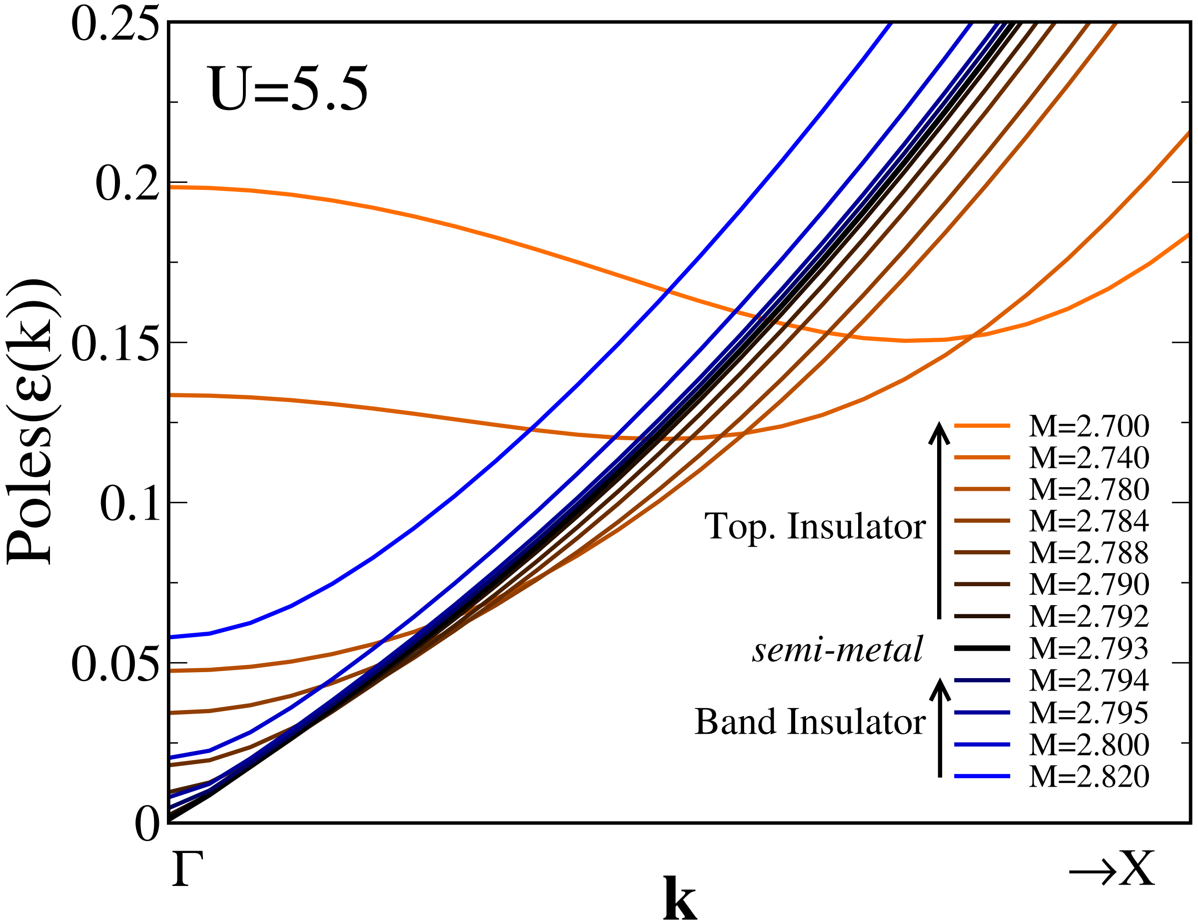




Signature of the 1st-order character:

Hysteretic behavior of the total energy, metastable states, coexistence.

Absence of gap closure



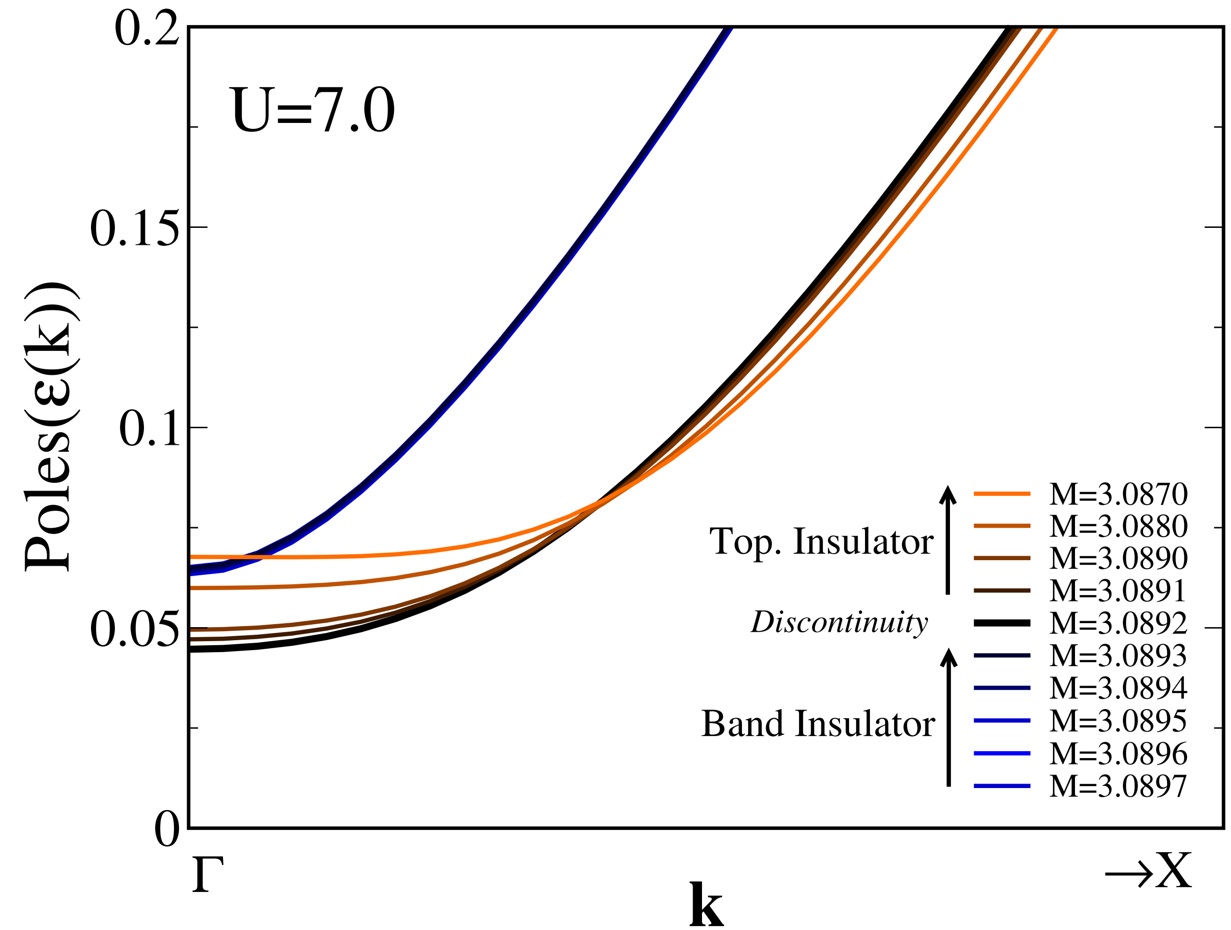
U<U$_c$: the transition to a topological state occurs in the usual band-gap closing way.

Dirac cone (*gapless*) at the transition.

U>U$_c$:

No gap-closing

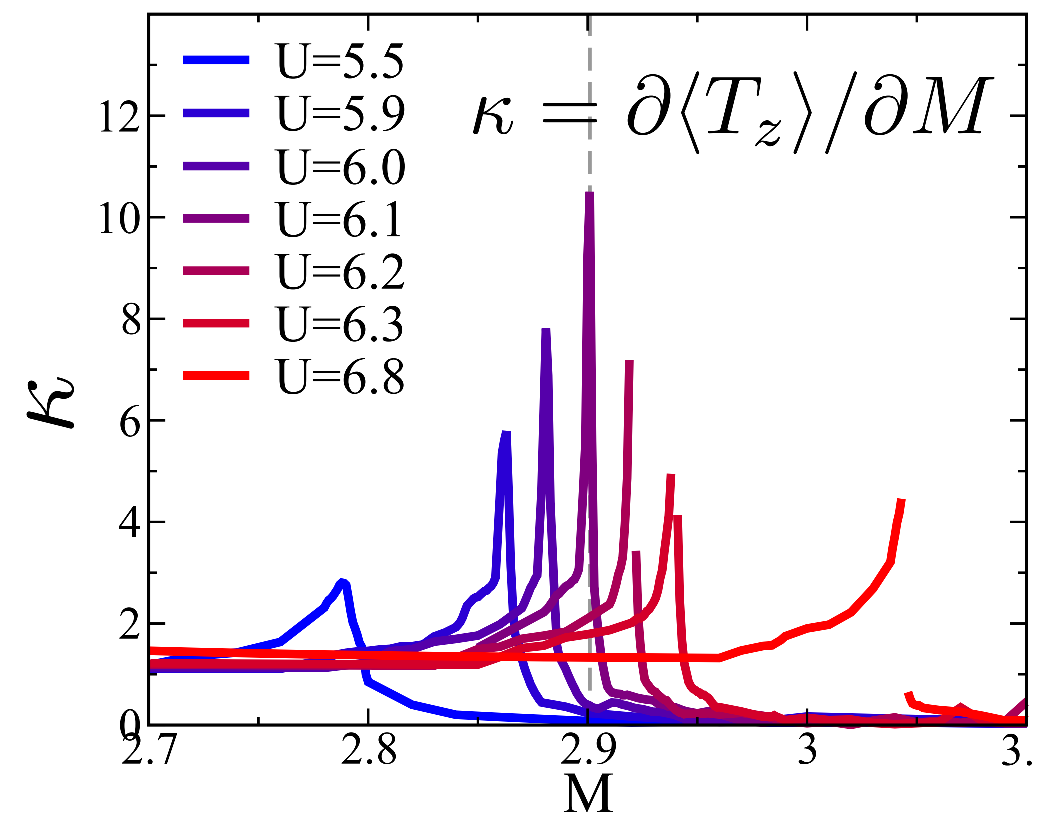
No suppression of any symmetries connected to the topological ordering.



Experimental signatures.

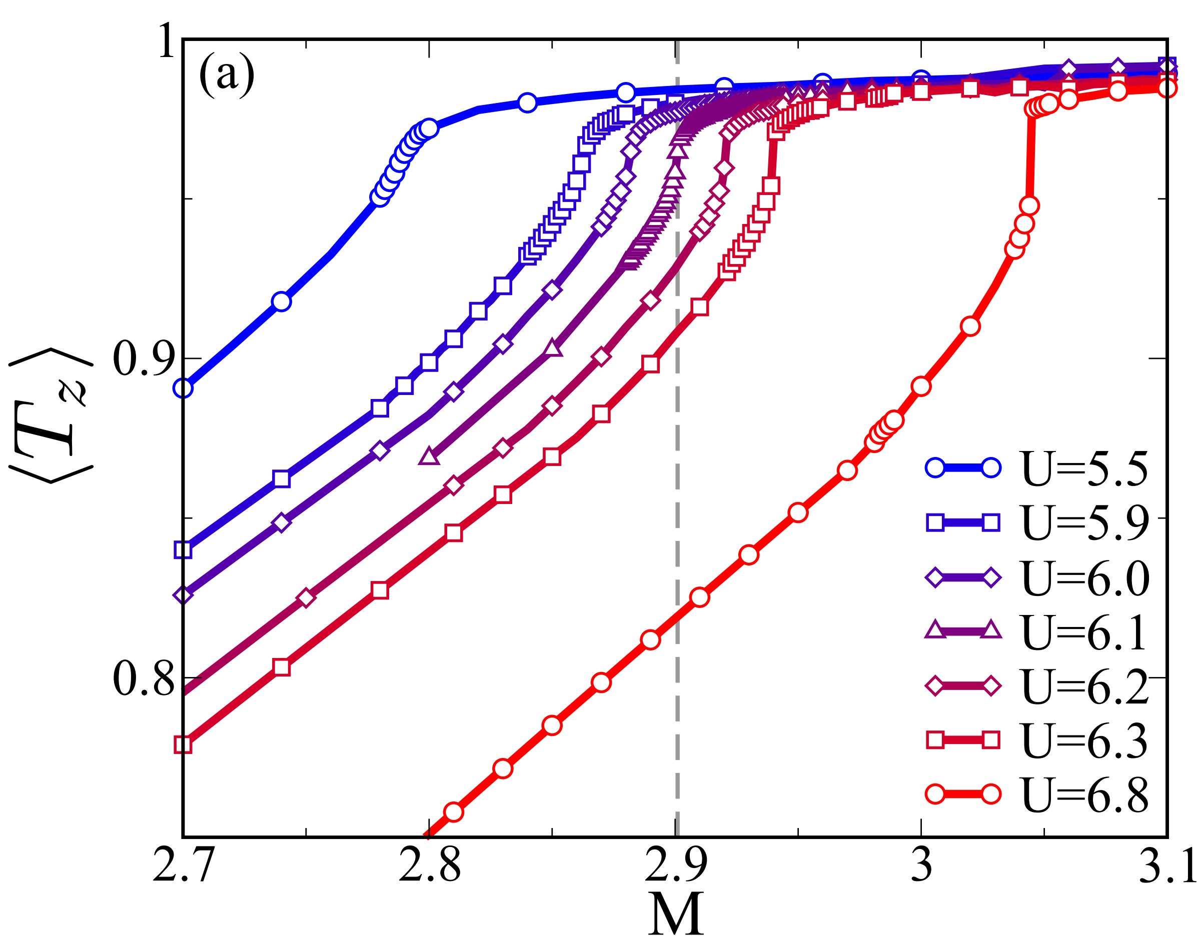
Like liquid and gas become distinguishable at low-T only…

Clearcut experimental distinction between trivial and non-trivial phase.



Instability in the orbital sector

Diverging orbital compressibility at $U=U_c$



Critical orbital polarization T_z

diverging fluctuations at the QCP

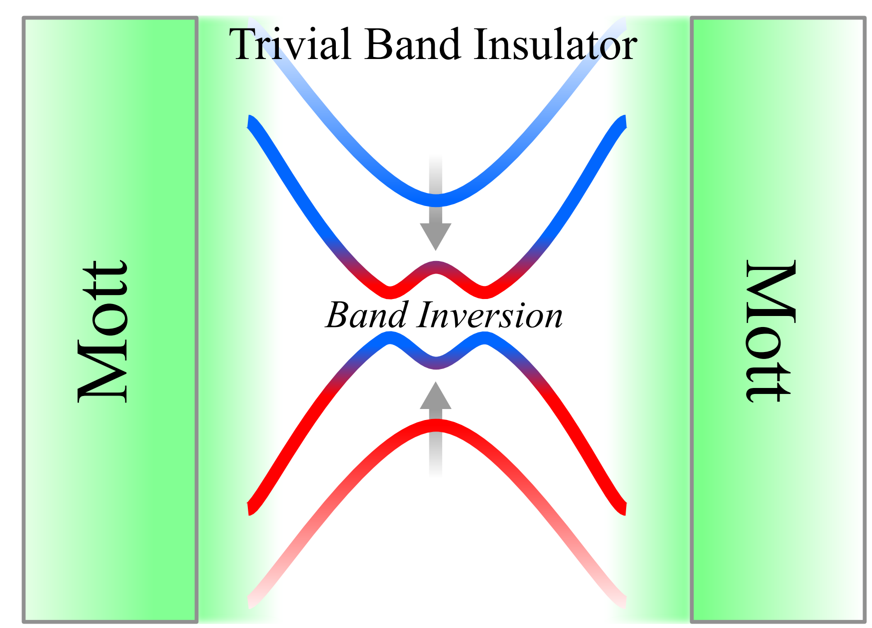
Experimental accessible quantities marking the topological phase-transition.

Conclusions.

- Interaction driven QSHI states.
- Emergent thermodynamic character: 1^{st} order transition.
- Topological QPT with NO gap closing & no-symmetry breaking!
- Experimental signatures of TQPT in correlated materials.

Outlook & Works in Progress…

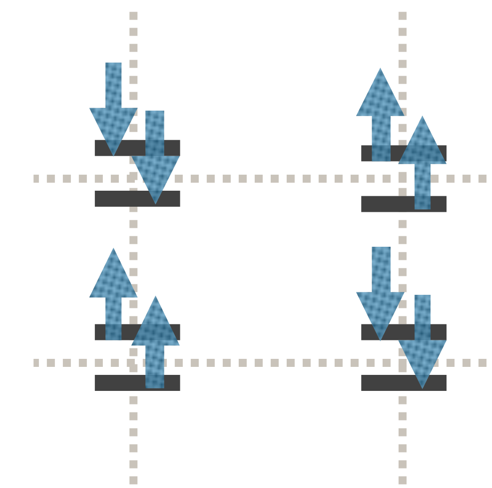
- Real materials with ab-initio + DMFT.
- Engineer a correlated QSH state.
- **Breaking SU(2)! Interacting Weyl Semi-Metals.**

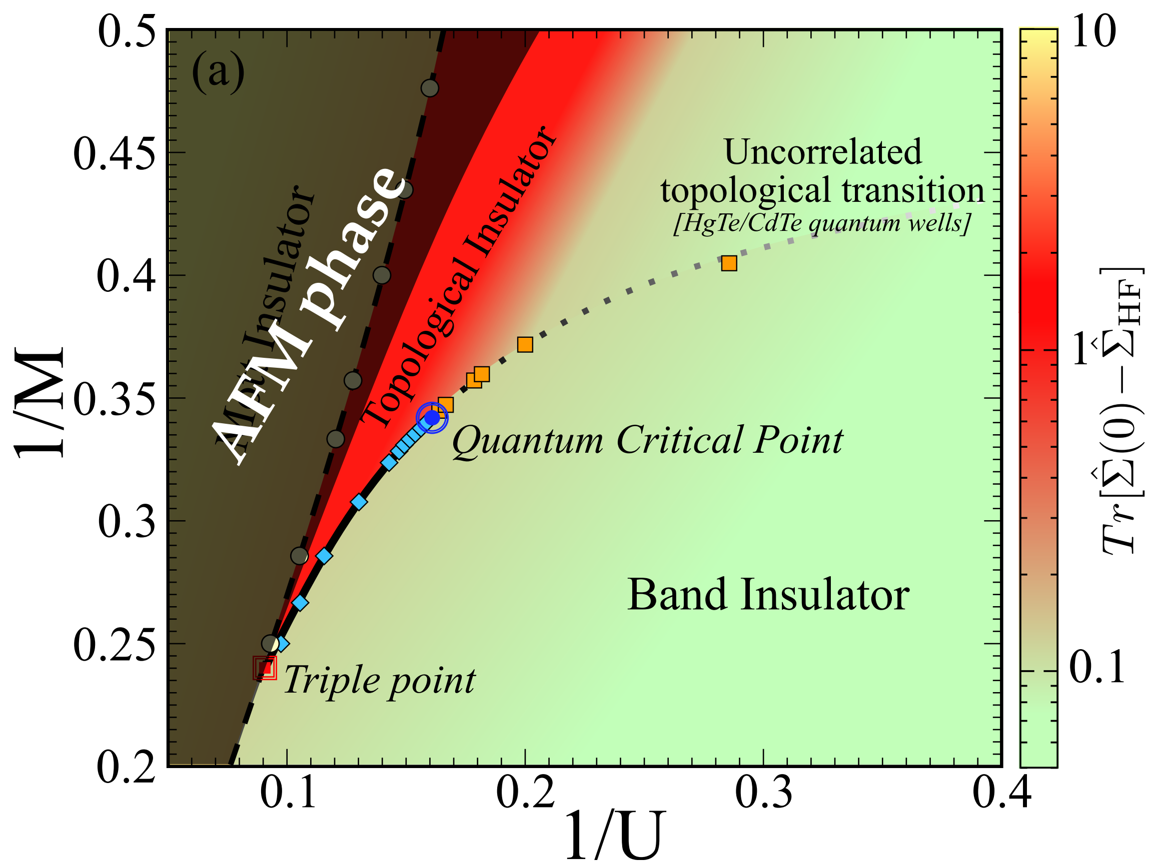


Anti-ferromagnetic order

Large local moments: unstable to magnetic order.

AFM "g-type" phase in proximity of the Mott Insulator.



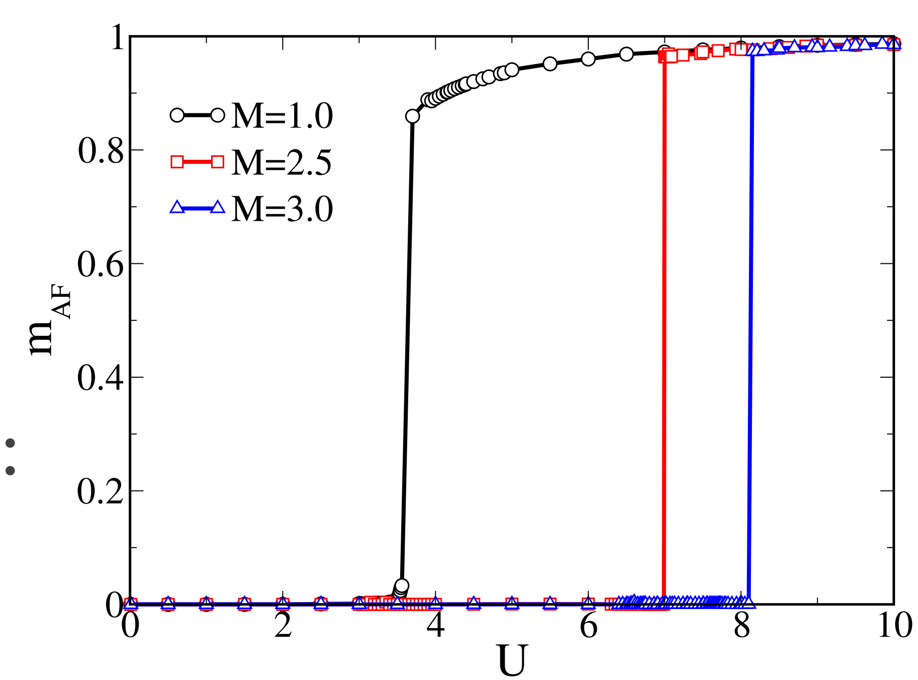


Ordered phase competes with TI.

Correlated-QSHI robust against AFM.

No traces of non-trivial AFM.

At T=0 AF magnetisation shows a large jump: 1st order transition.

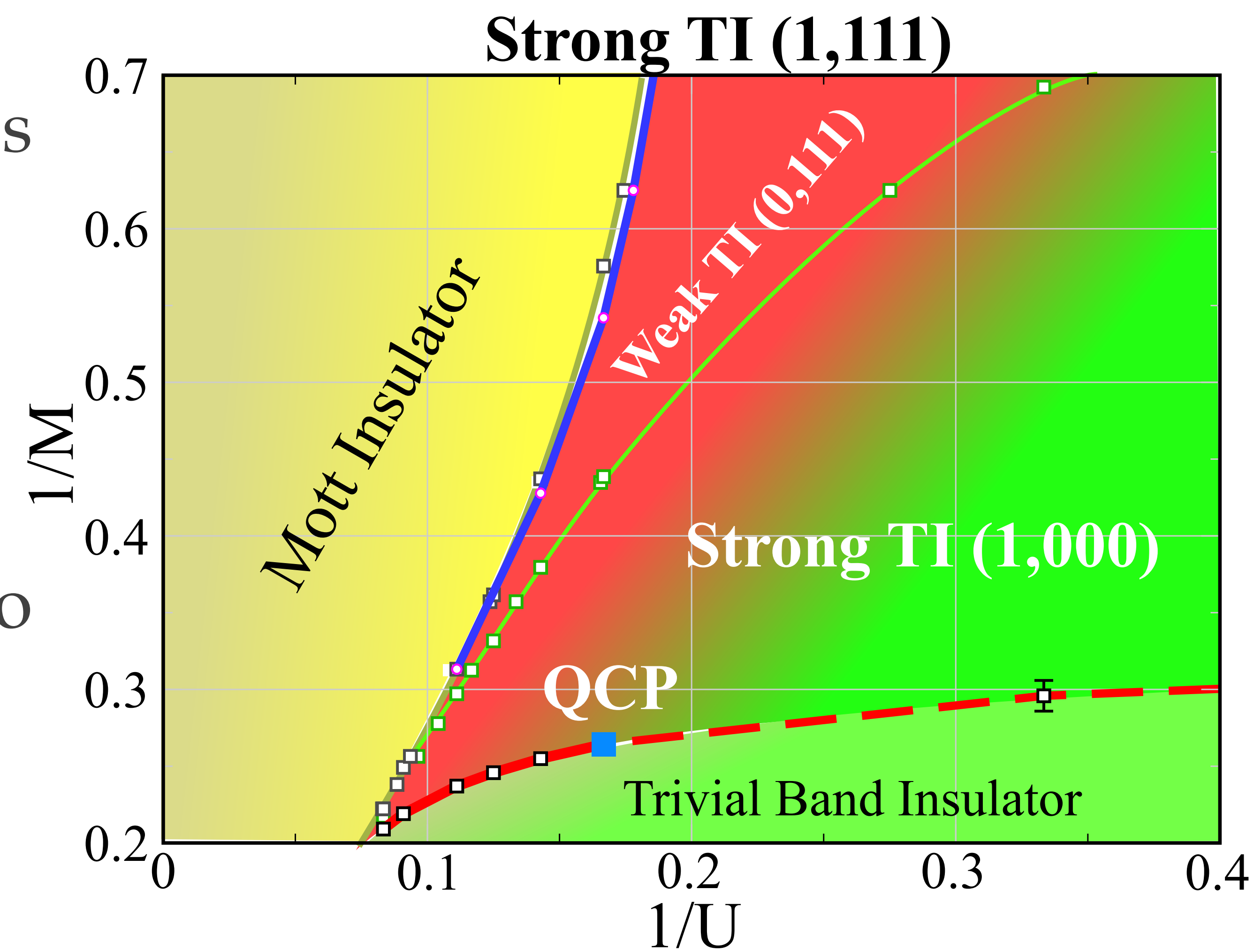


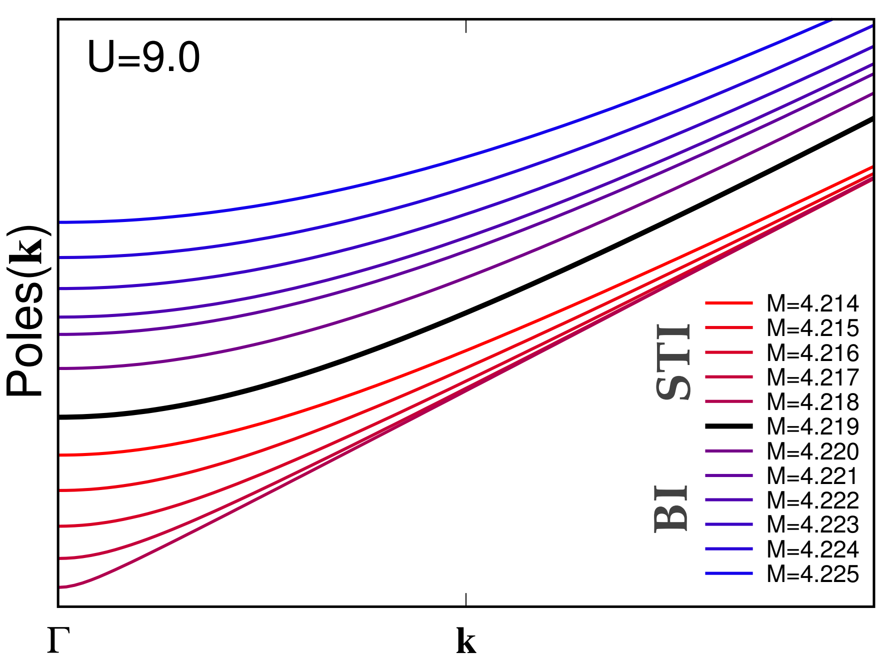
Generalisation to 3D

Quantum Critical Point dominates physics also in the 3D case.

1st-order transition to **Strong TI**

Anomalous STI (1,111) preludes to Mott transition.





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