Strong correlation effects in 2D topological quantum phase transitions

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Frontiers in 2D Quantum Systems, ICTP

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Dresden

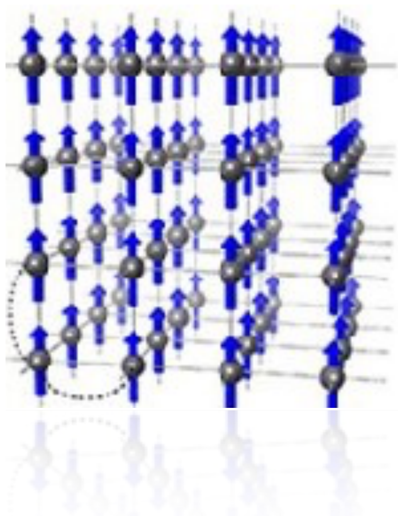
J. Budich

Introduction.

Ginzburg-Landau theory: *symmetry breaking* classification of matter phases

key concept: ***local order parameter***

Magnetism

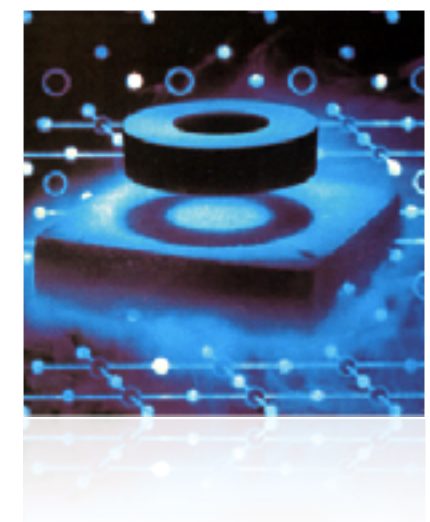


magnetization M

Liquid-gas

density difference n(L)-n(G)

"Superconductivity"



pair amplitude ψ

Experimental detectability!

Introduction.

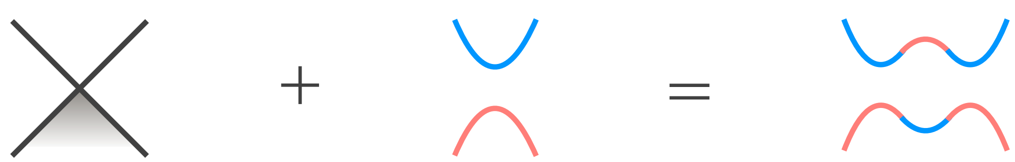
Haldane PRL88
Kane,Mele PRL05
Bernevig et al Science 2006
…. many more

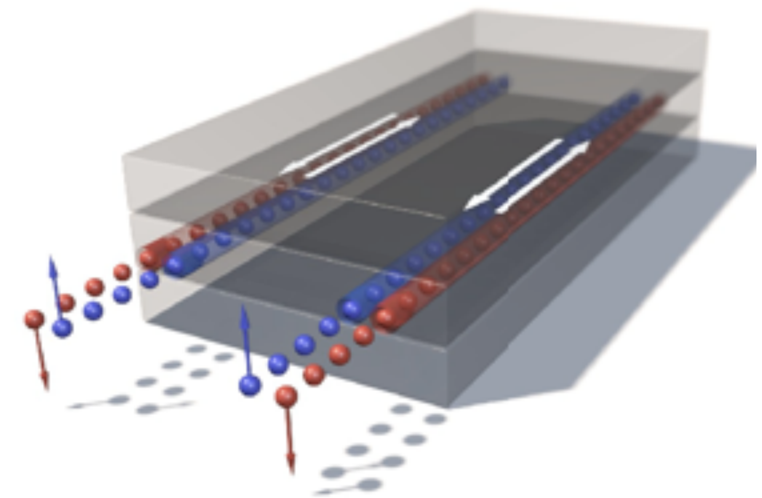
TOPOLOGICAL INSULATORS

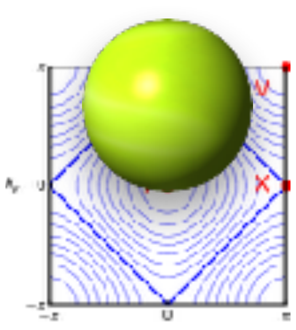
quantum materials eluding the G-L paradigm!

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

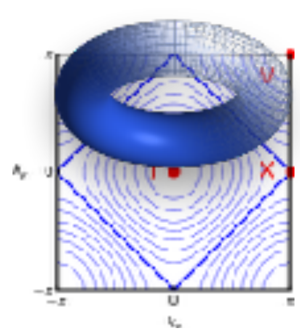
Dirac semi-metal + *Spin-Orbit Coupling*





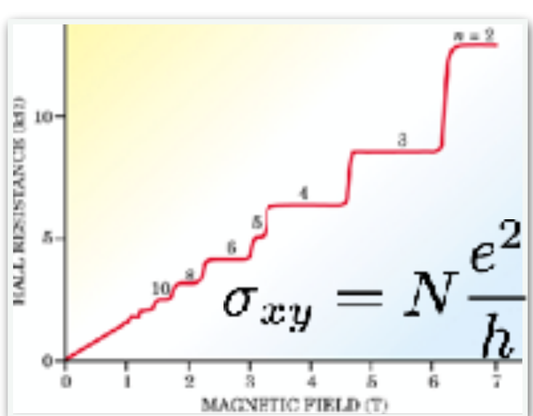


Trivial



Non-Trivial

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



key concept: ***global topological invariant***

The 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

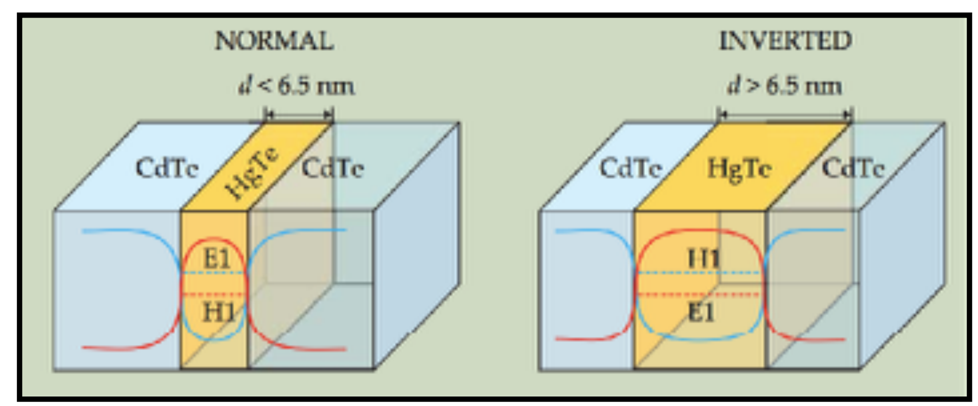
BHZ model: *2 QHI + Time Reversal Symmetry.*

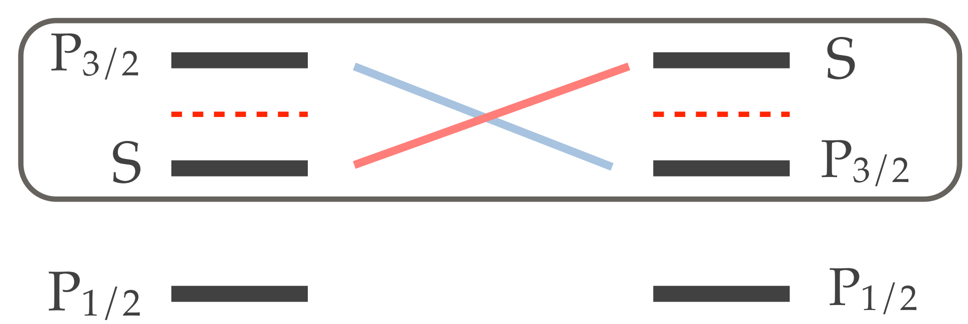
CdTe/HgTe **quantum wells.**

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

$$\mathbf{h}(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \tau$$ *Orbital pseudo-spin structure*

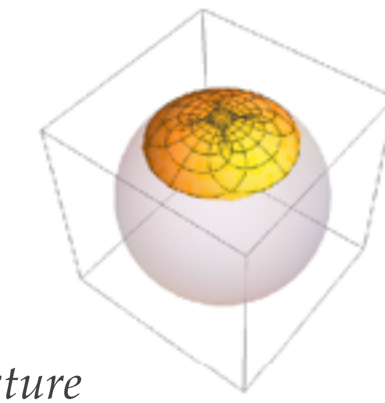
$$\mathbf{d}(\mathbf{k}) = [\lambda \sin k_x, \lambda \sin k_y, M - \varepsilon(\mathbf{k})]$$





Topological QPT

$\mathcal{C}_1=0$



spin texture

M> 2

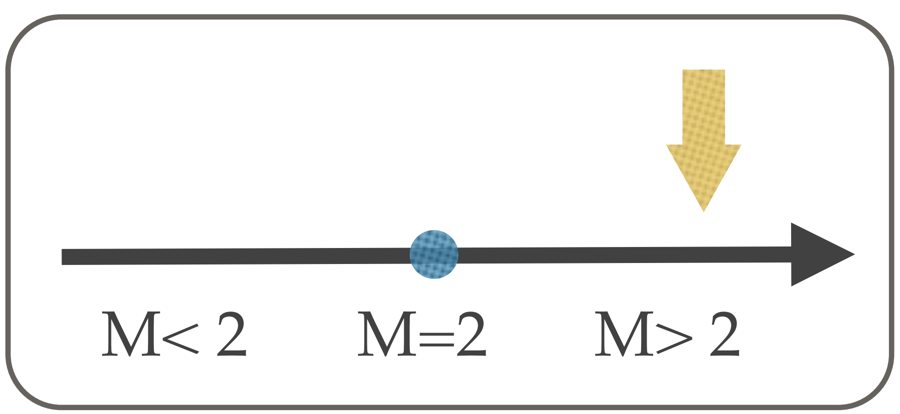
$\mathbf{d}(\mathbf{k})$

BHZ description of topological transition:

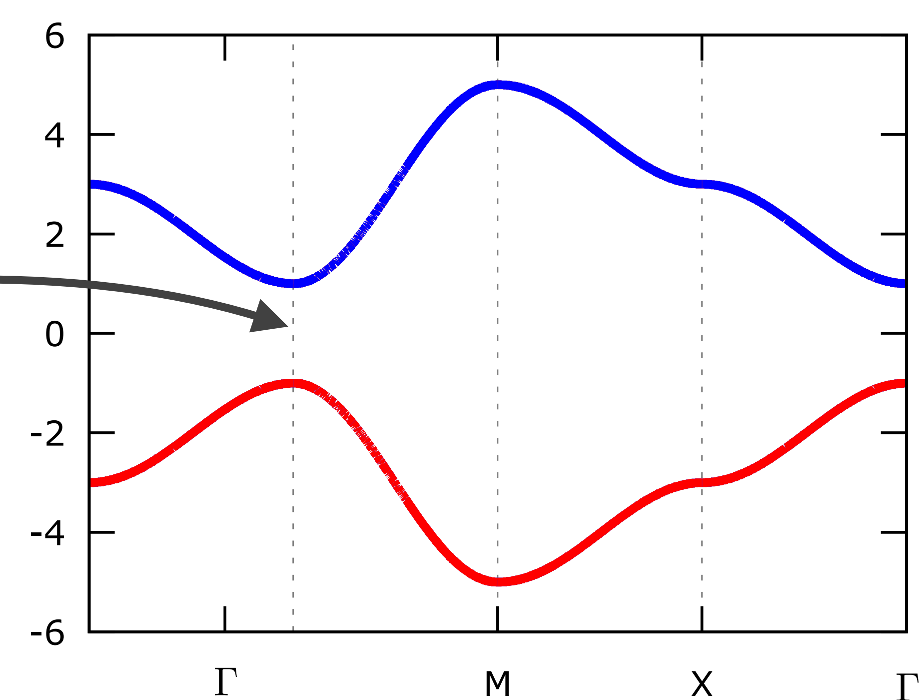
$$\mathbf{h}(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \tau$$

Continuous Topological Quantum Phase Transition

band structure evolves smoothly with control parameters…



trivial band insulator



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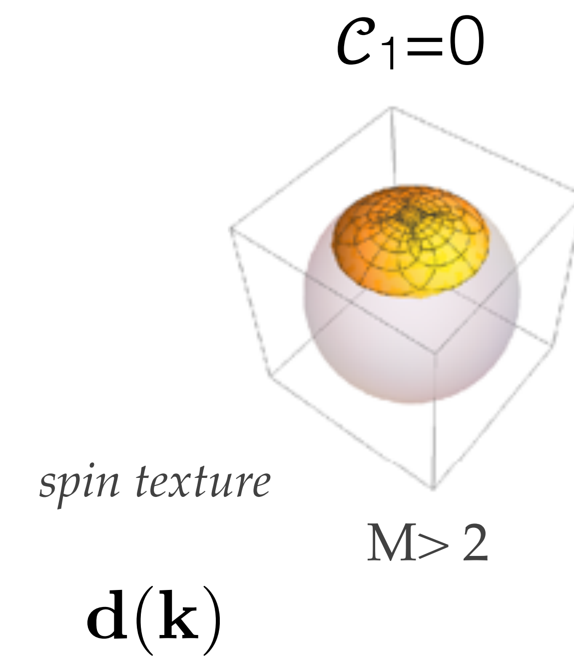

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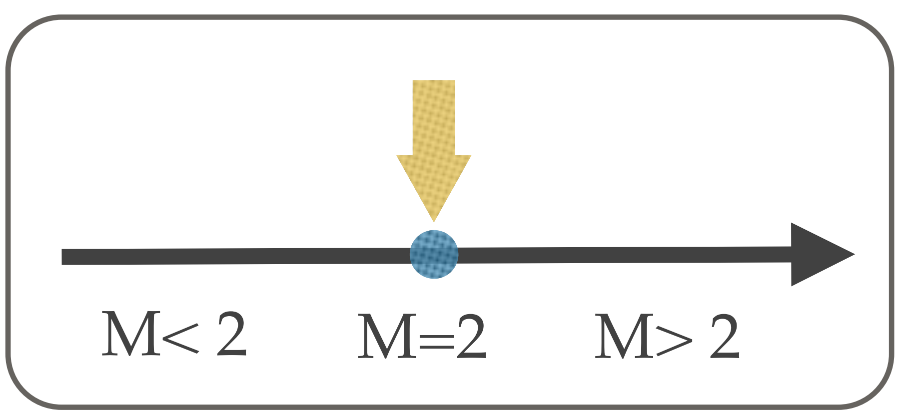
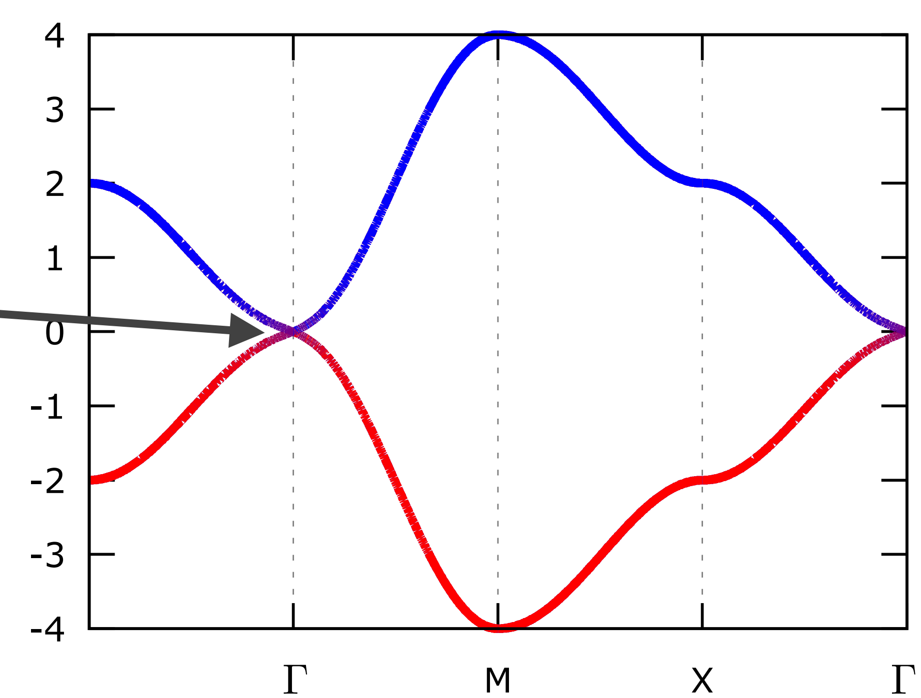


Dirac cone semi-metal



Topological QPT

BHZ description of topological transition:

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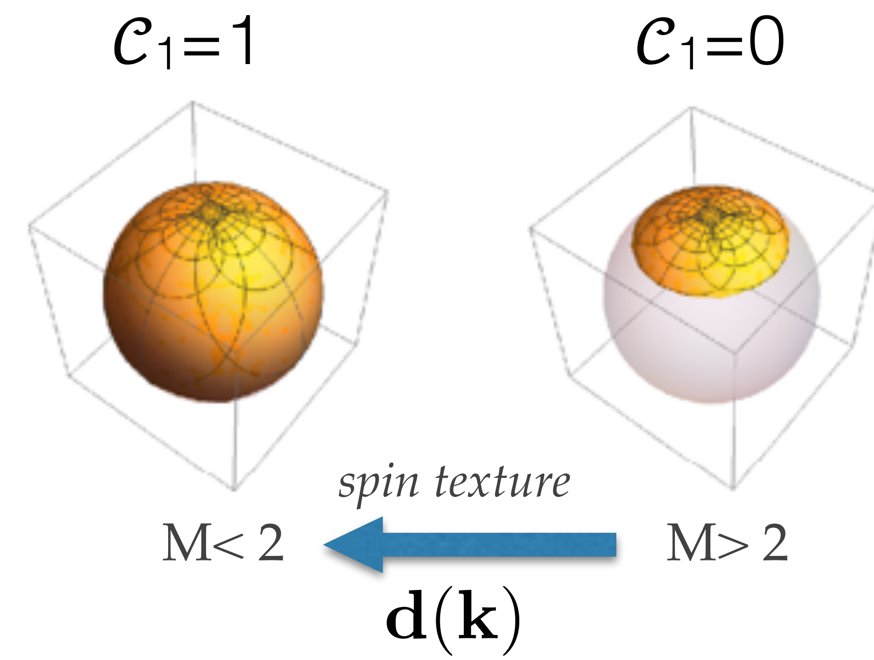

Continuous Topological Quantum Phase Transition

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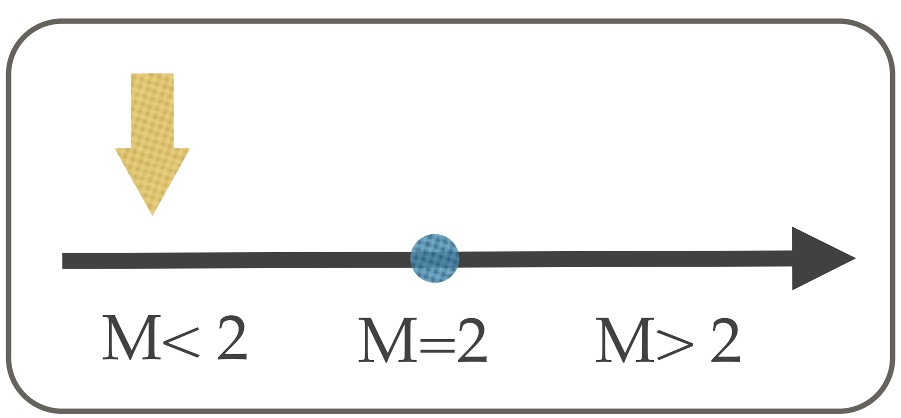
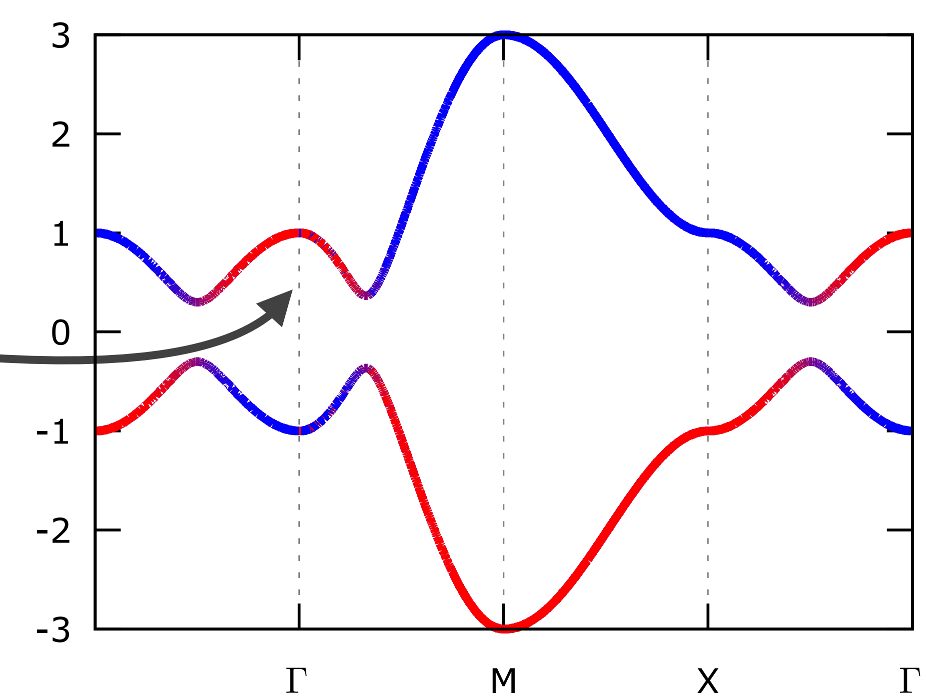
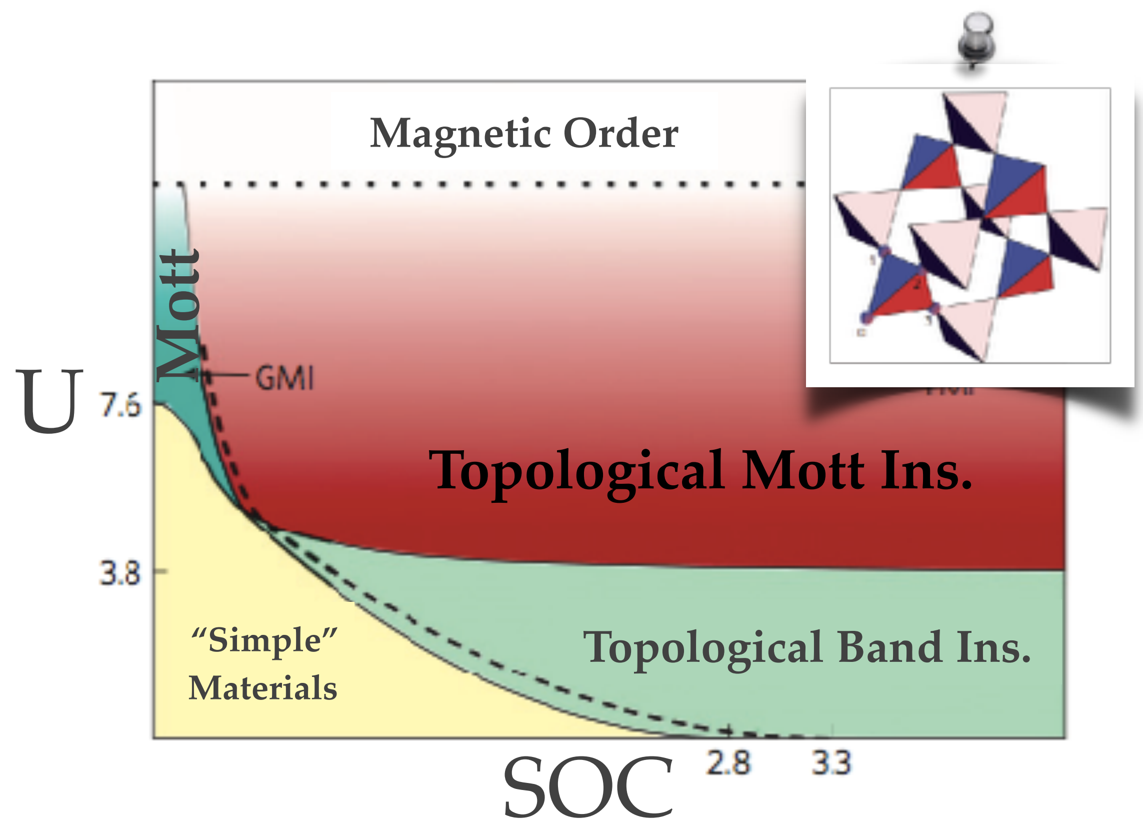


band inversion
QSH insulator



What about the interaction?

Quest for larger SOC…heavy elements compounds (*5d/4,5f*)



Hexaborides ***Sm/Pu***B_6,

Ir-based pyrochlores: $Sr_2\mathbf{Ir}_2O_7$ *, etc..*

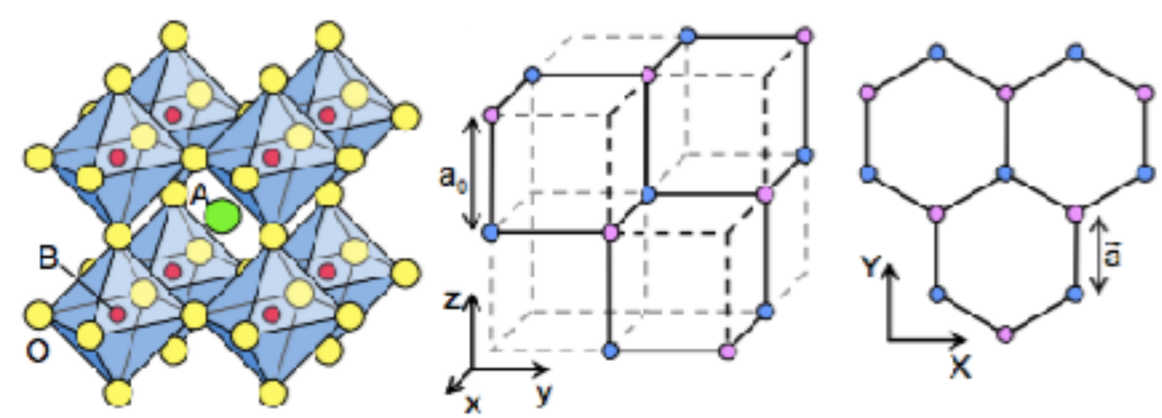
Dzero et al. PRL 2010
D. Pesin, L. Balents, NP 2010
Hohenadler , Assad. Journal of Phys. 2013
Deng et al PRL 2013

New materials?

Engineering correlated TI:

Transition Metal Oxides Heterostructures

D. Xiao et al. Nat. Comm. 2011



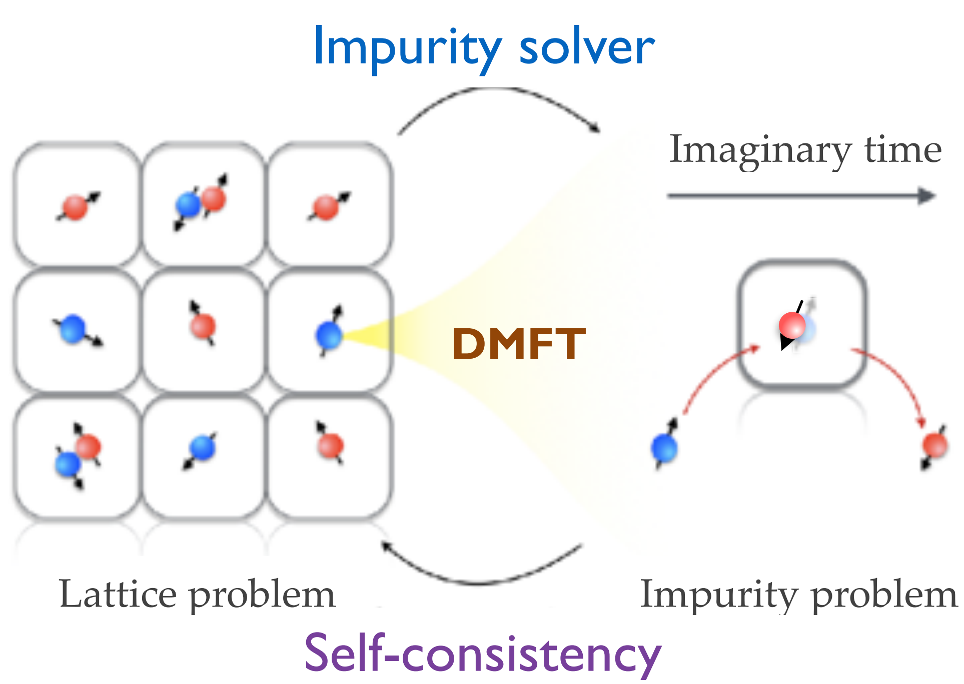
$LaAuO_3$

DMFT solution

Dynamical Mean-Field Theory

<u>non-perturbative solution of the interacting problem</u>

Idea: Reduce the interacting lattice problem to a *self-consistent* impurity problem



Advantages:

+ local quantum physics *(beyond Hartree-Fock)*.
+ non-perturbative in the interaction
+ access to topological invariant

Drawbacks:

- neglects spatial fluctuations
- computational demanding…

solve using **Exact Diagonalization** & **CTQMC**

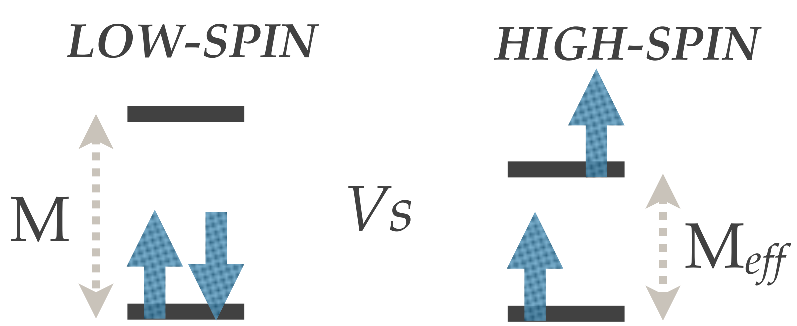
Obtain *dynamical* (non-scalar) self-energy.
Describes the effects of interaction.

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

BHZ - Interaction

AA et al PRL 2015
AA et al PRB 2016

BHZ effective minimal model + multi-orbital interactions

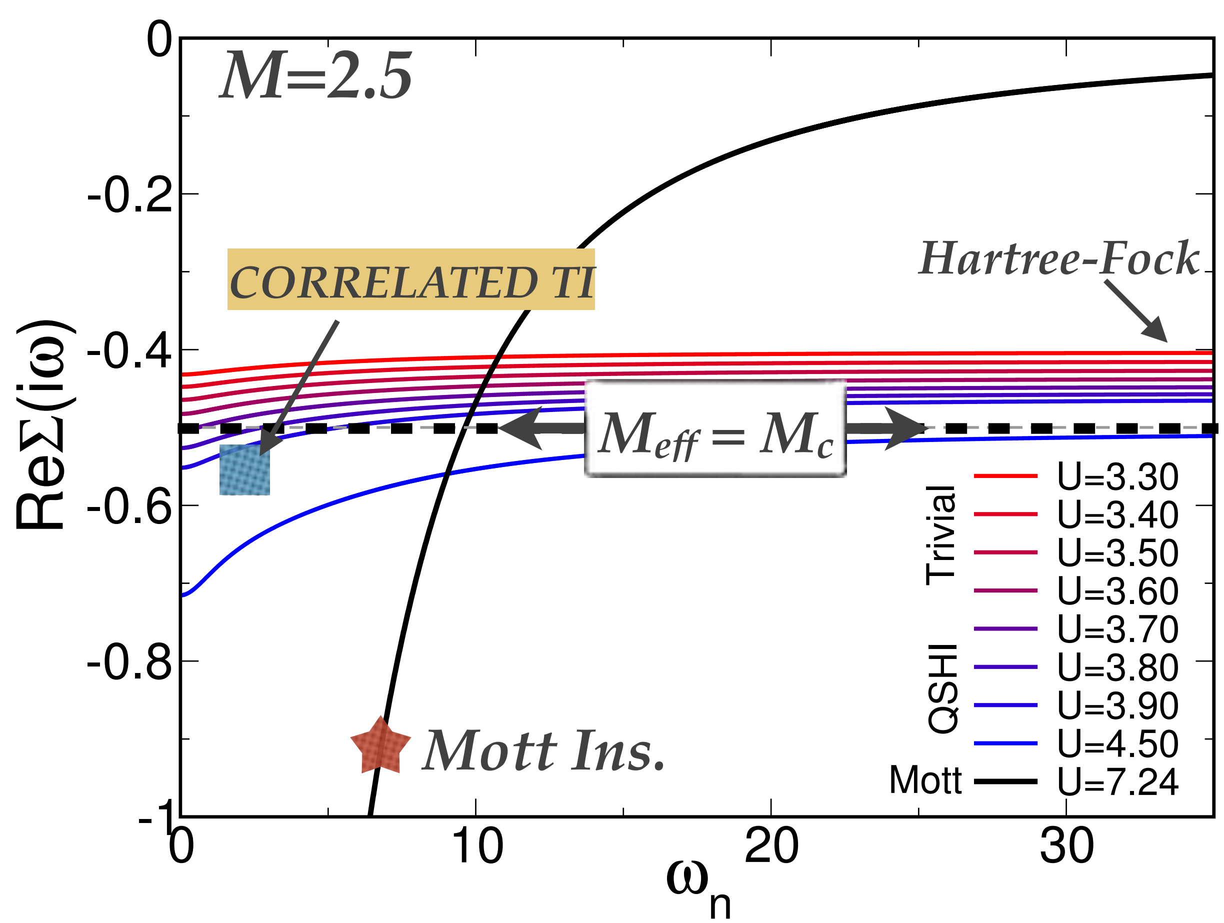


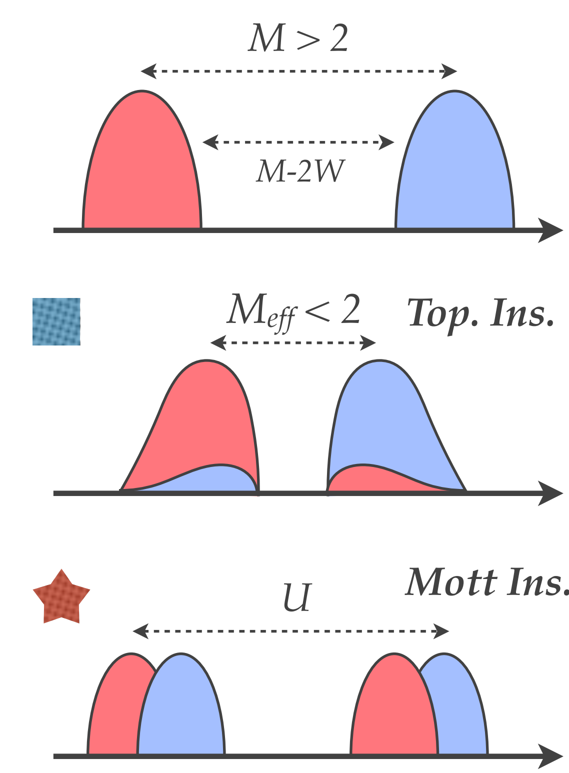
$$H_I = (U - J_H)\frac{N(N-1)}{2} - J_H\left(\frac{N^2}{4} + \frac{S_z^2}{2} - 2T_z^2\right)$$

Effective reduction of the Mass term: $M_{\rm eff} = M + {\rm Tr}[\tau_z \hat{\Sigma}(0)]/2$

Interaction driven **TI**

Mott phase at large U



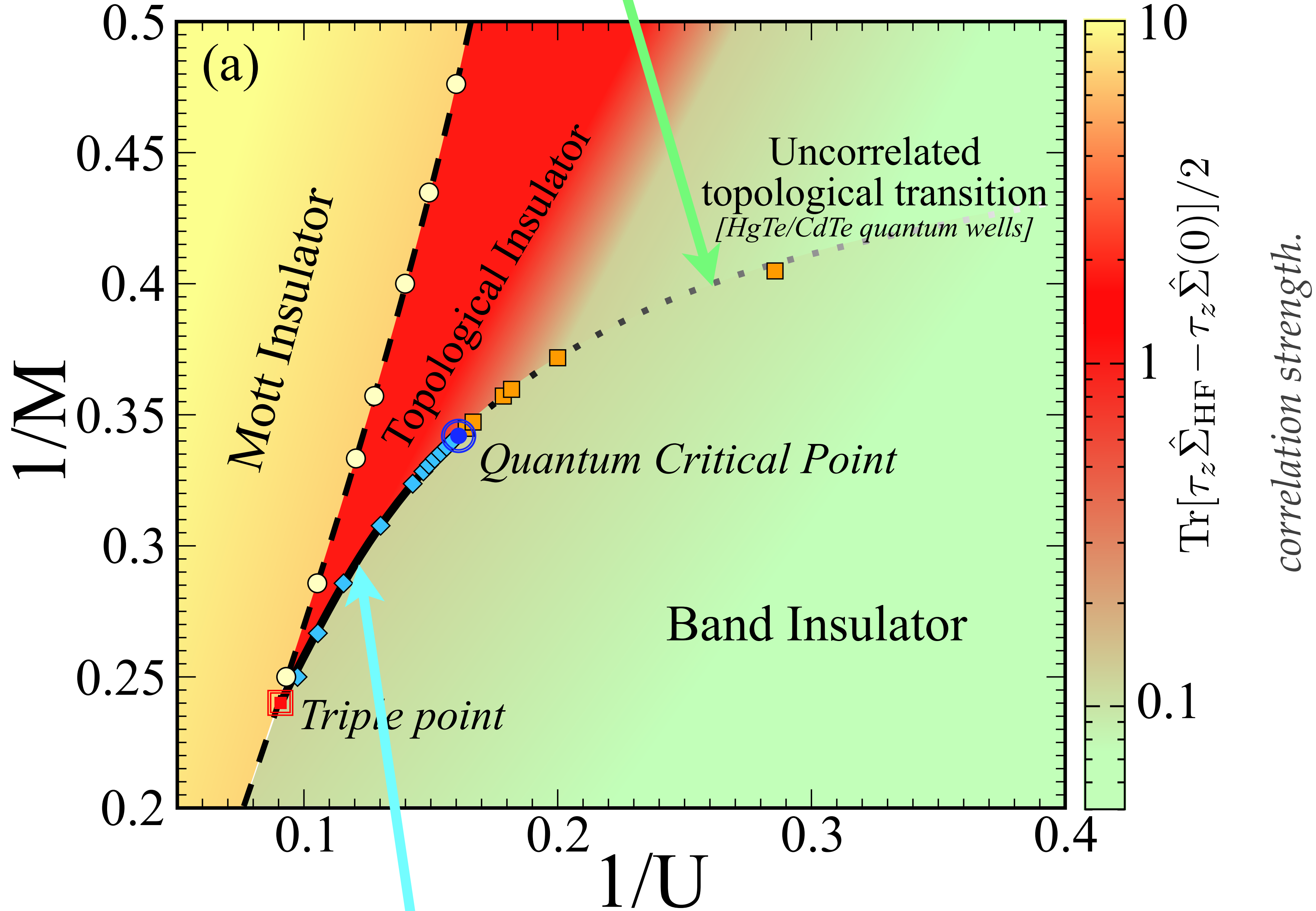


Correlated QSHI

AA et al PRL 2015

Phase diagram M-U (*flipped view*).

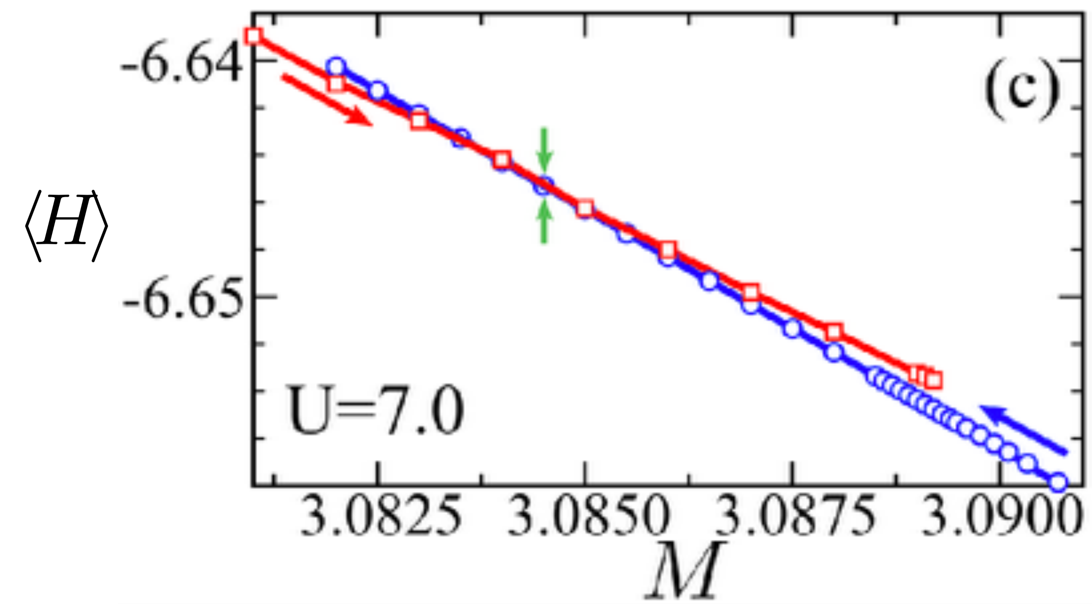
Weak coupling: ***Continuous*** ~ U=0



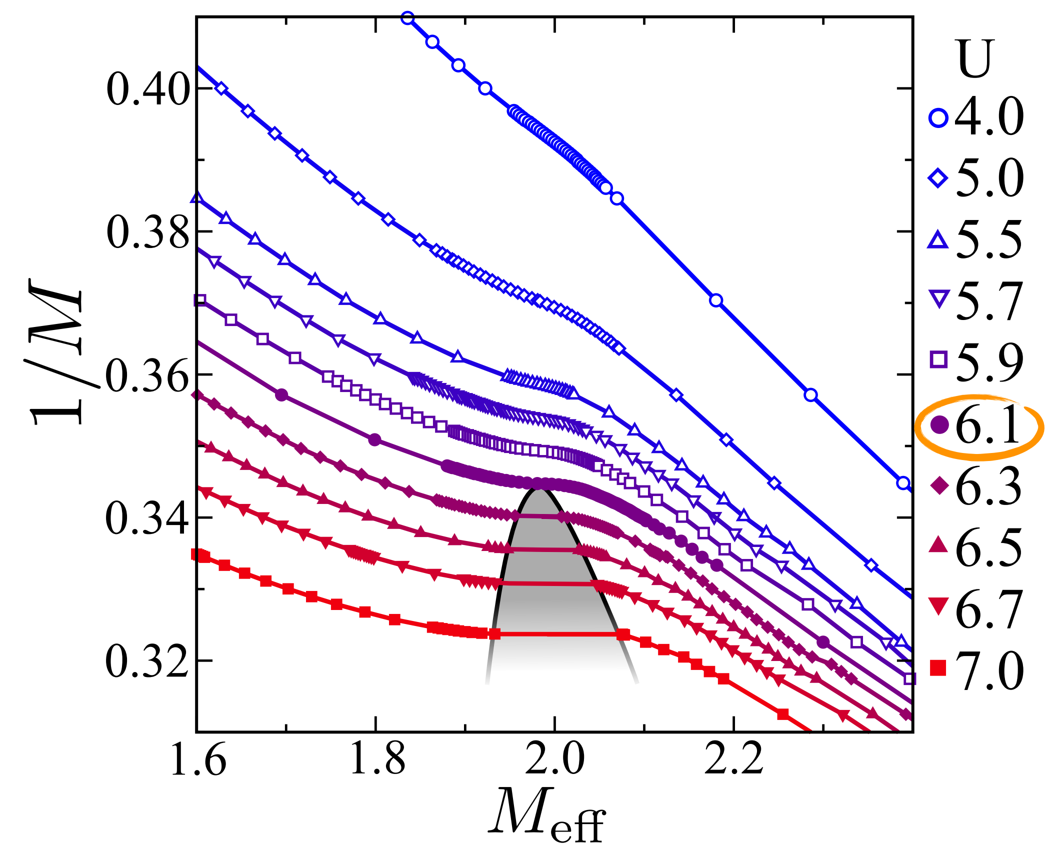
Strong coupling: 1st order TQPT correlated many-body character

Correlated QSHI

AA et al PRL 2015

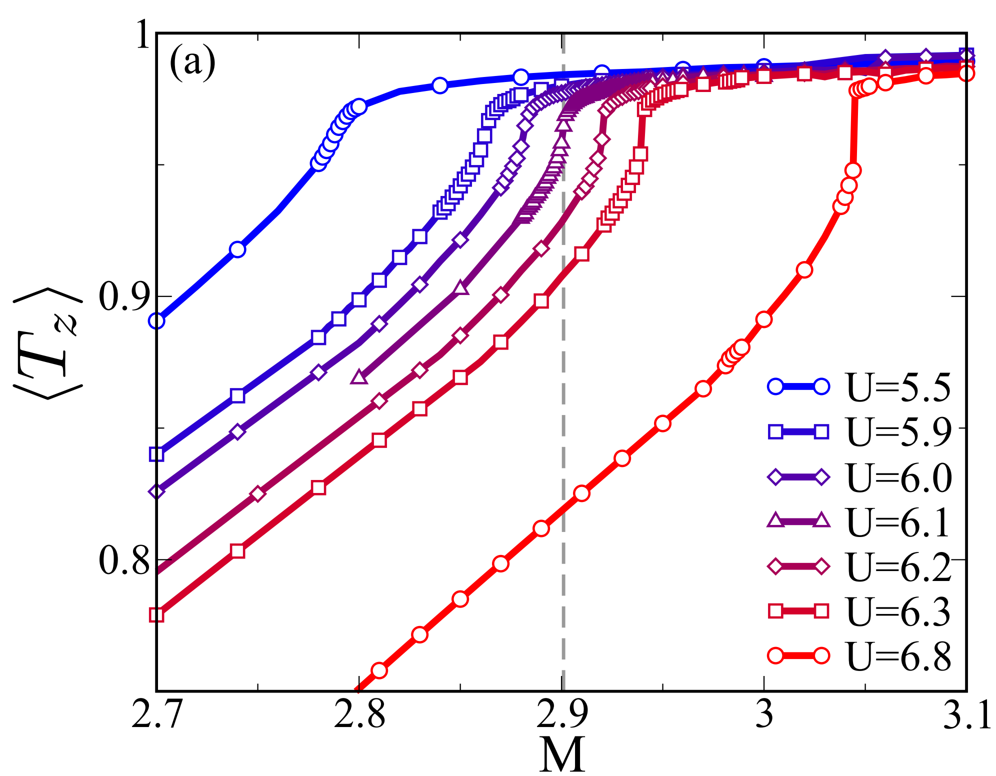


Metastable states hallmark of 1st transition.



A clear picture from the *iso*-U curves

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



Diverging orbital compressibility at $U = U_c$

$$\kappa = \partial \langle T_z \rangle / \partial M$$

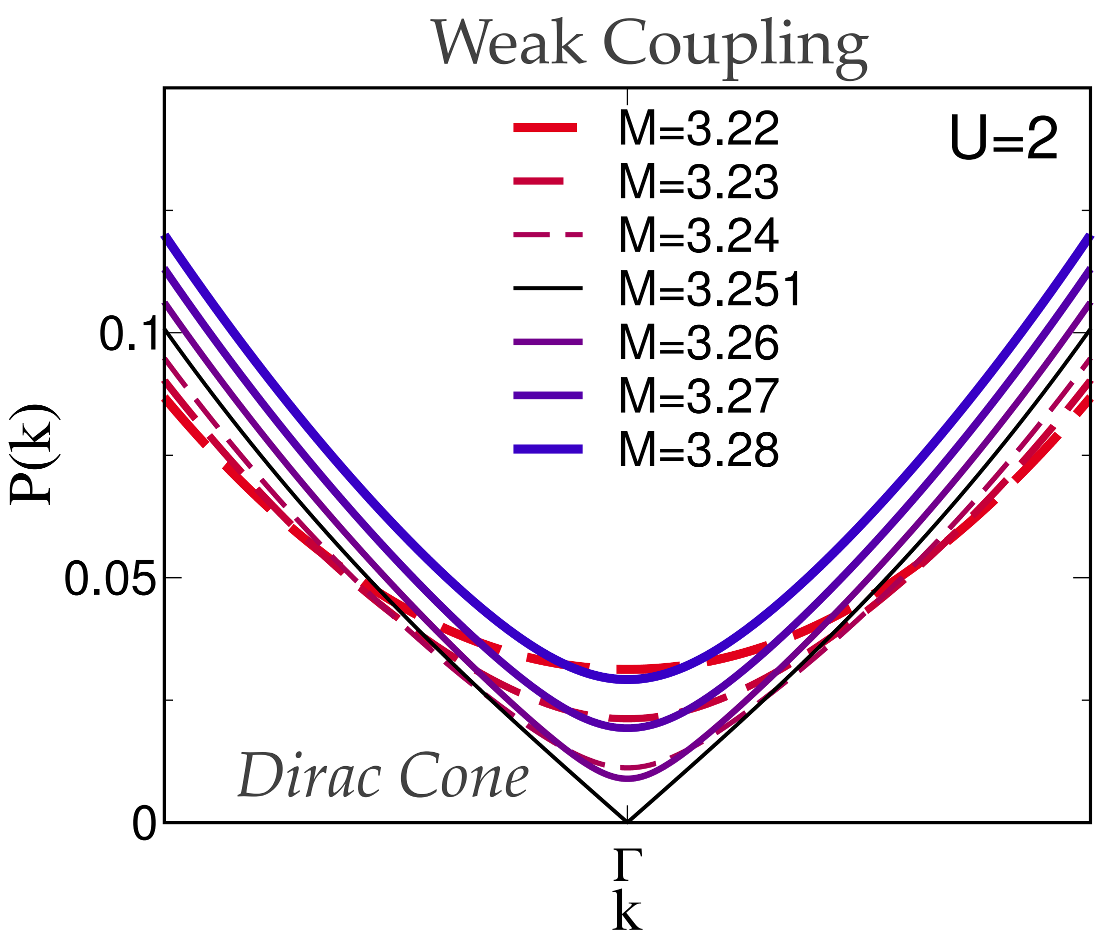
Experimental accessible quantities marking the TQPT.

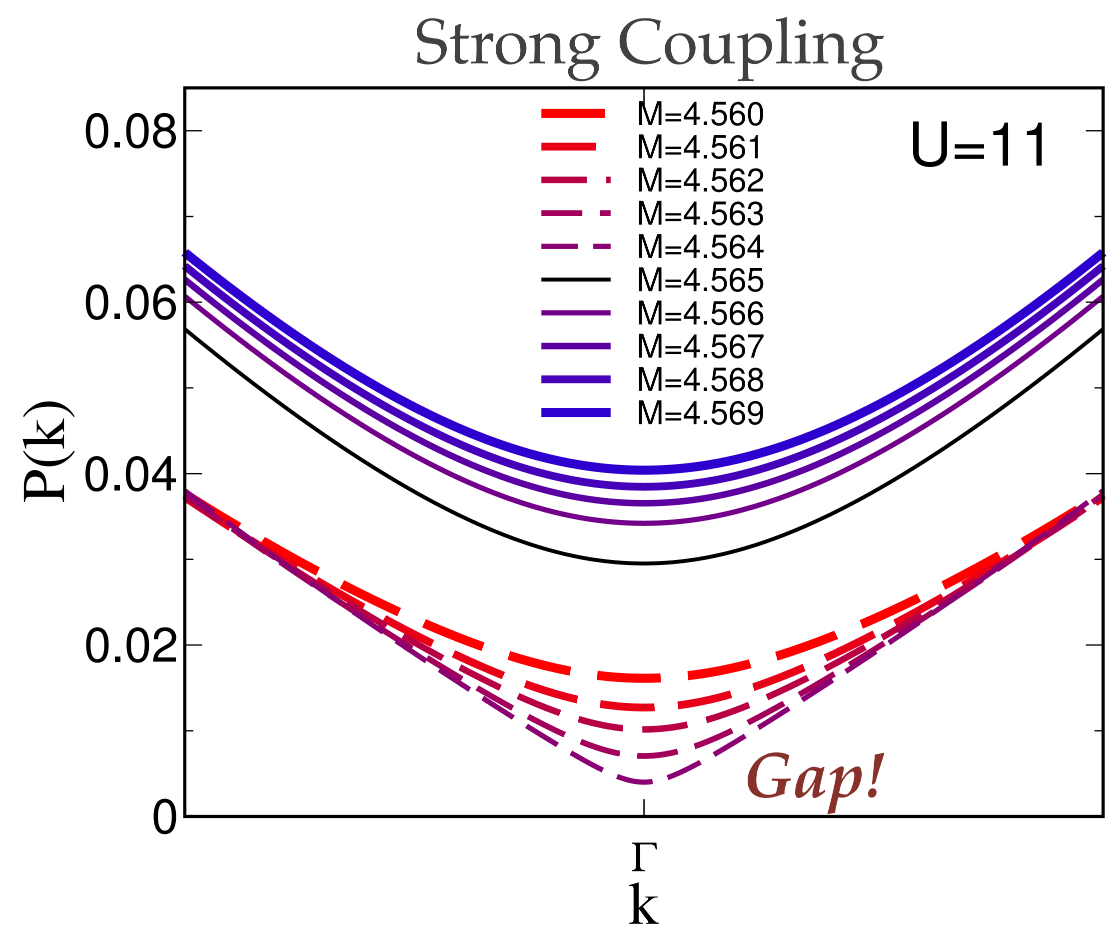
Absence of gap closure

AA et al PRL 2015

AA et al PRB 2016

Breakdown of the gap-less TQPT paradigm…





$U<U_c$

The transition to a topological state occurs thru band-gap closing.
Dirac cone formation.

$U>U_c$

No gap-closing

No suppression of any symmetries protecting the topological state.

Correlated edge states

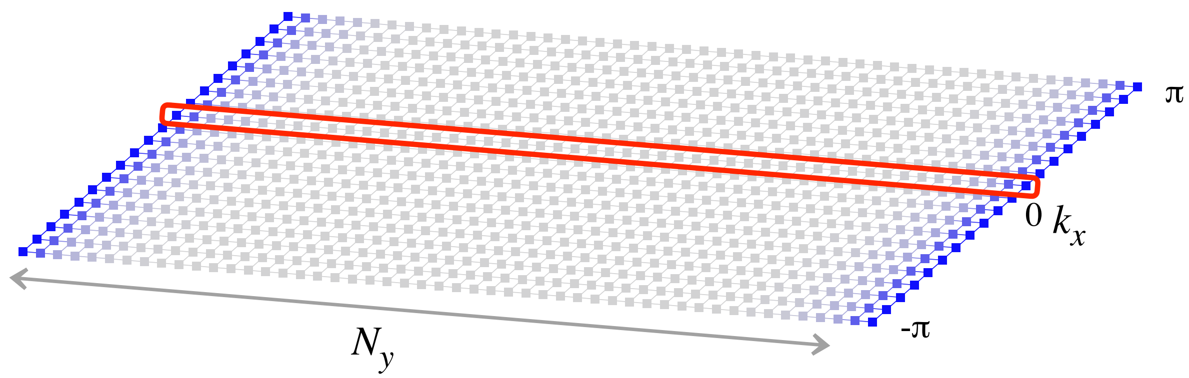
AA et al. PRB 2017

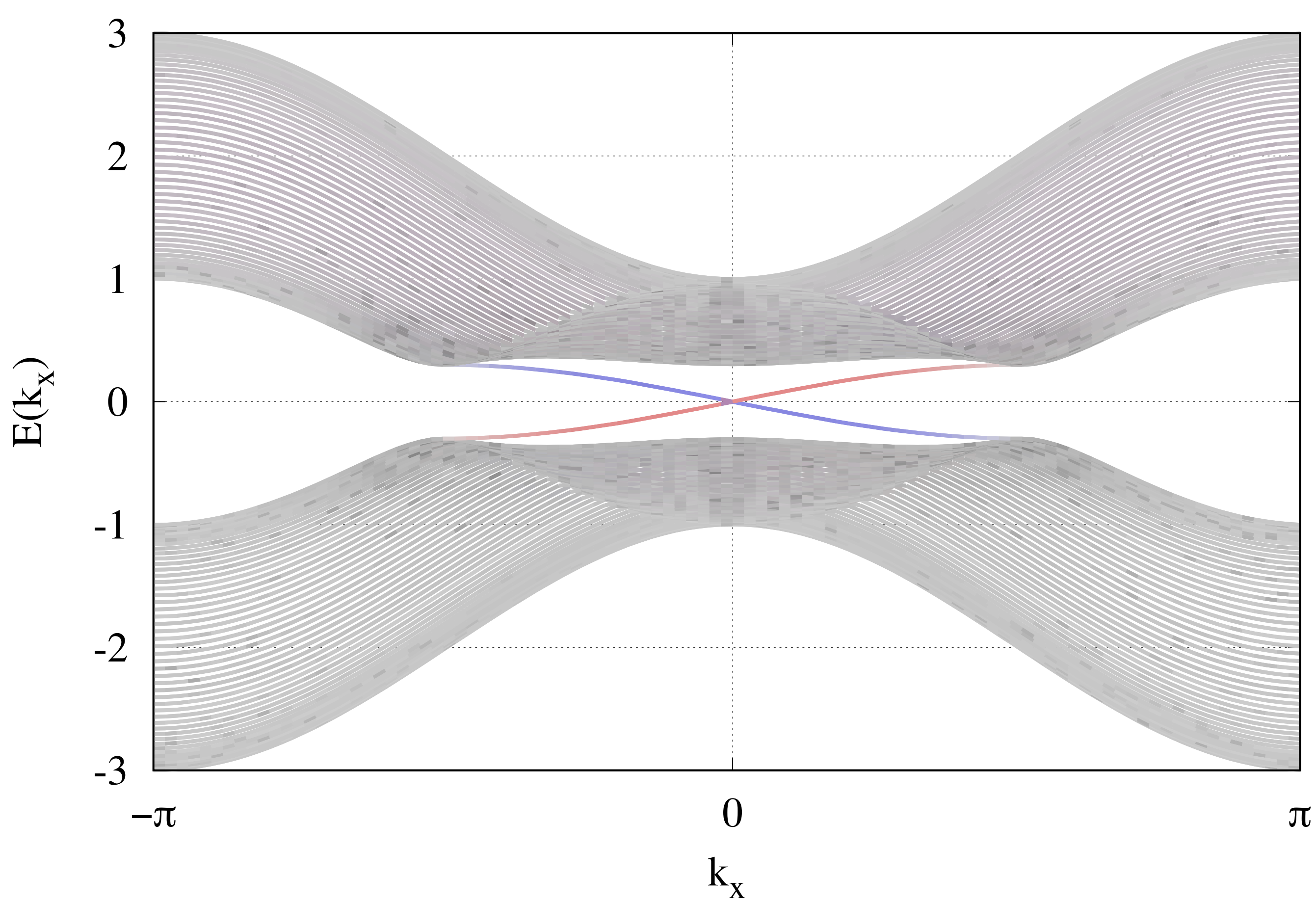
Consider a 2D stripe.

$$H = \sum_{k_x yy'} \Psi^{+}_{k_x y} \mathbf{M}(k_x) \delta_{yy'} \Psi_{k_x y'} + \sum_{k_x yy'} \left(\Psi^{+}_{k_x y} \mathbf{T} \delta_{y+1 y'} \Psi_{k_x y'} + H.c. \right)$$

$$\mathbf{M} = [M - 2t \cos k_x]\Gamma_5 + \lambda \sin k_x \Gamma_x$$

$$\mathbf{T} = -t\Gamma_5 + i\frac{\lambda}{2}\Gamma_y$$





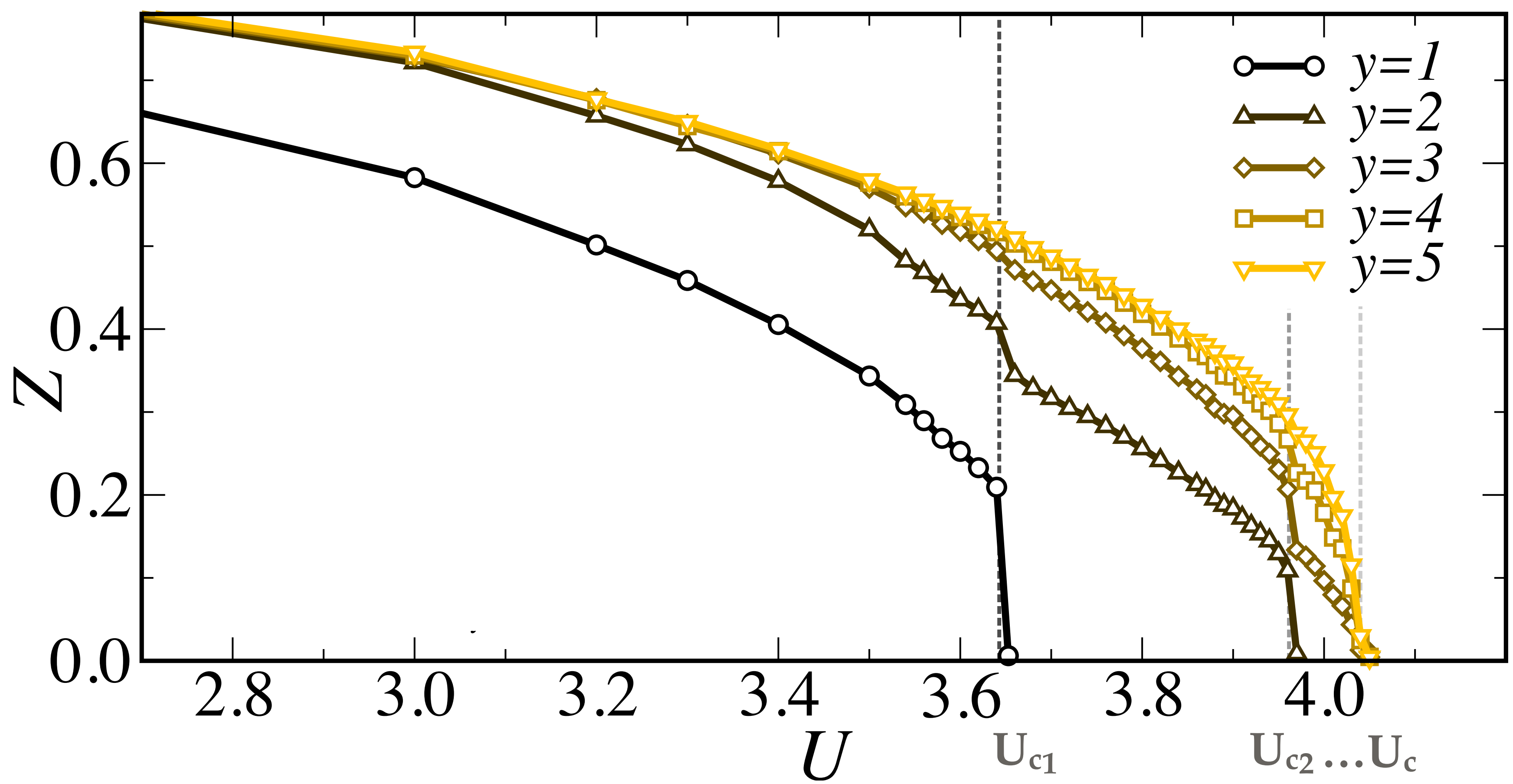
Helical gapless states localized at the edges.

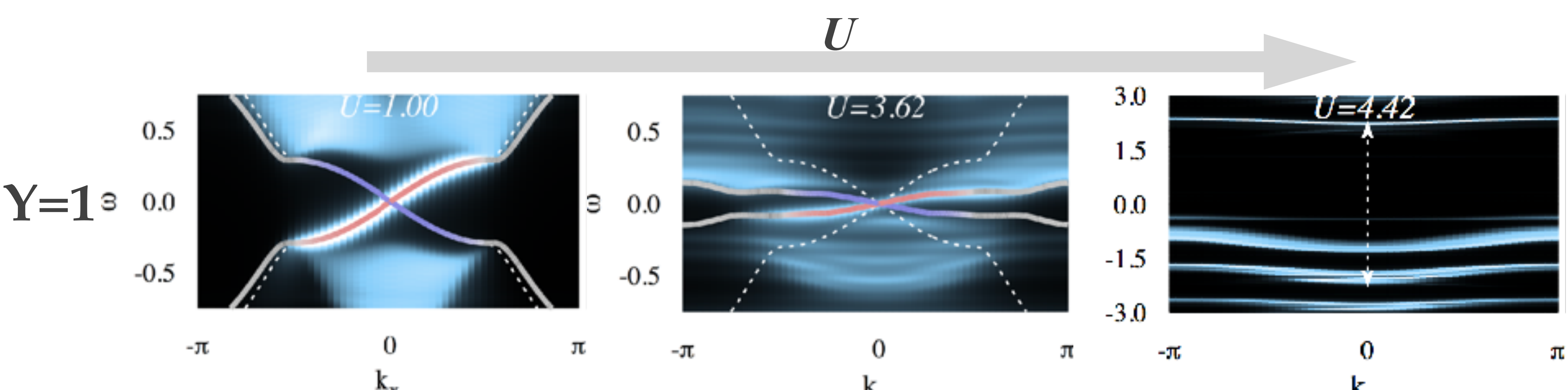
What's the effects of strong correlation on the 2D stripe?

Correlated edge states

AA et al. PRB 2017

Sequence of transitions to reach the Mott state.



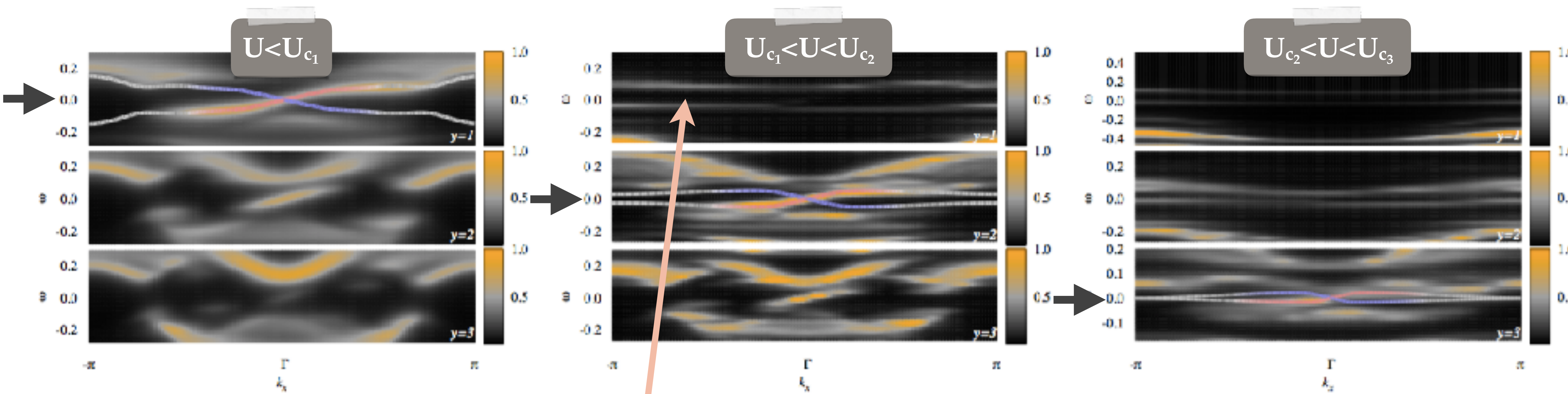


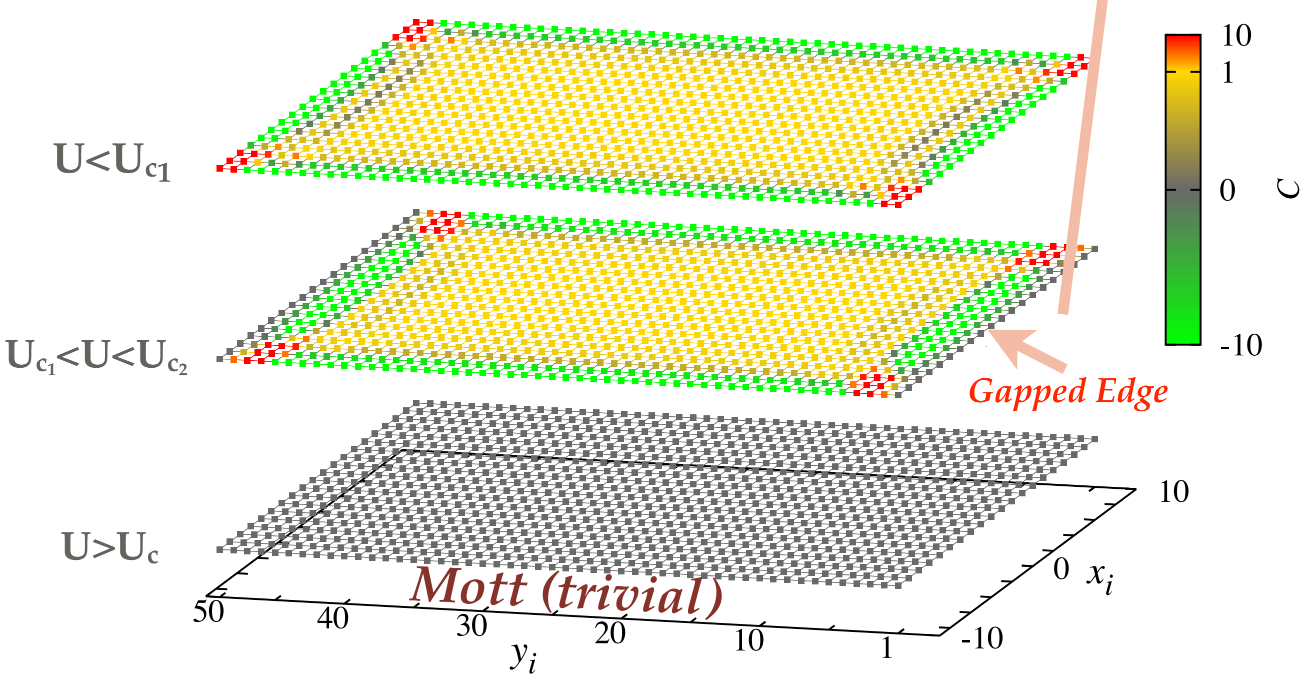
Correlated edge states

***AA** et al. PRB 2017*

What's the fate of the edge states?

Bulk compression —> Edge state reconstruction





Topological properties with OBC:

Local Chern Marker

$$\mathfrak{C}_\sigma(\mathbf{r}) = 2\pi i \langle \mathbf{r} | \hat{x}^\sigma_{\mathcal{P}} \hat{y}^\sigma_{\mathcal{Q}} - \hat{y}^\sigma_{\mathcal{P}} \hat{x}^\sigma_{\mathcal{Q}} | \mathbf{r} \rangle$$

$$\mathbb{Z}_2 = (\mathcal{C}_\uparrow - \mathcal{C}_\downarrow)/2$$

Conclusions.

- Topological States can be favoured by strong interaction. ***AA*** *et al. PRL 2015* ***AA*** *et al. PRB 2016*
- *Emergent thermodynamic character*: 1st order transition.
- New paradigm for TQPT : **no** gap closing but **no** symmetry breaking!
- Correlation driven edge states reconstruction. ***AA*** *et al. PRB 2017* ***AA*** *et al. in preparation 2017*

Outlook...

- *Break TRS or IS:* ***correlation*** *effects in* ***Weyl SM****.*
- *Interplay of strong* ***interaction*** *and* ***SOC****: from models to real materials.*
- ***Topological Mott Insulators****.*
- *Condensed matter realization of excitations beyond "standard model"*