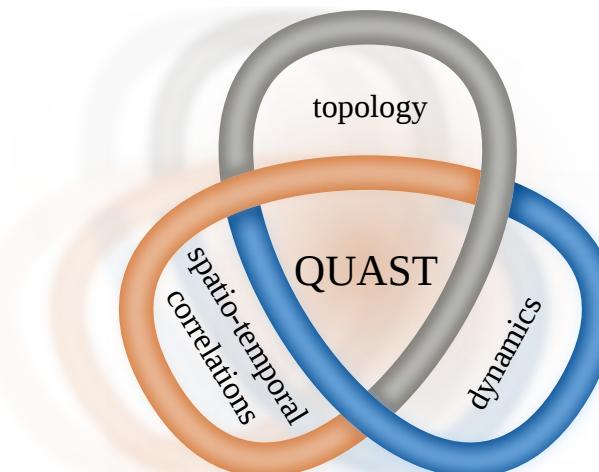


RPMBT XXI, Chapel Hill N.C., 12 Sep 2022

# Interacting Chern Insulator in Infinite Dimensions

Michael Potthoff  
University of Hamburg



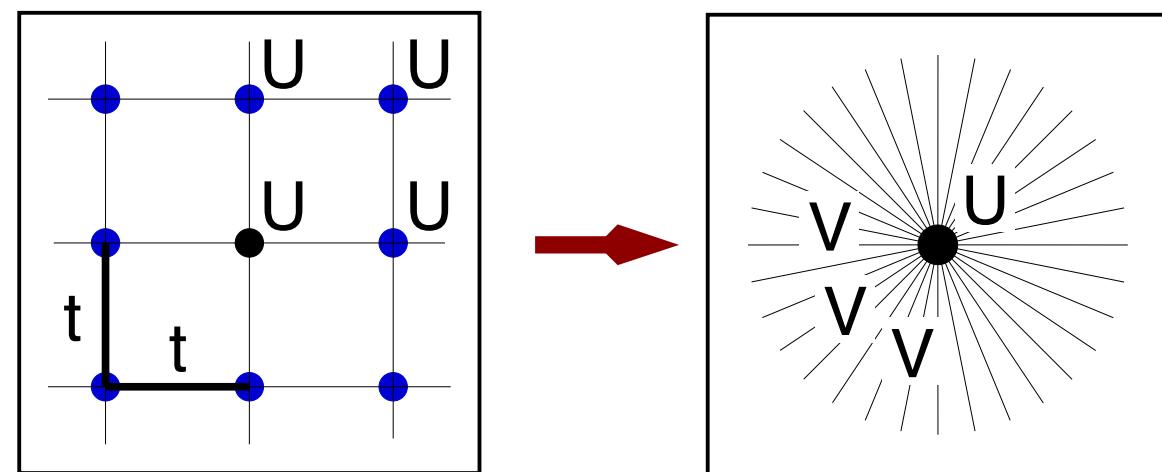
# Motivation



David Krüger  
University of Hamburg

## Frontiers of Condensed-Matter Theory

- strong electron correlations
- topological classification



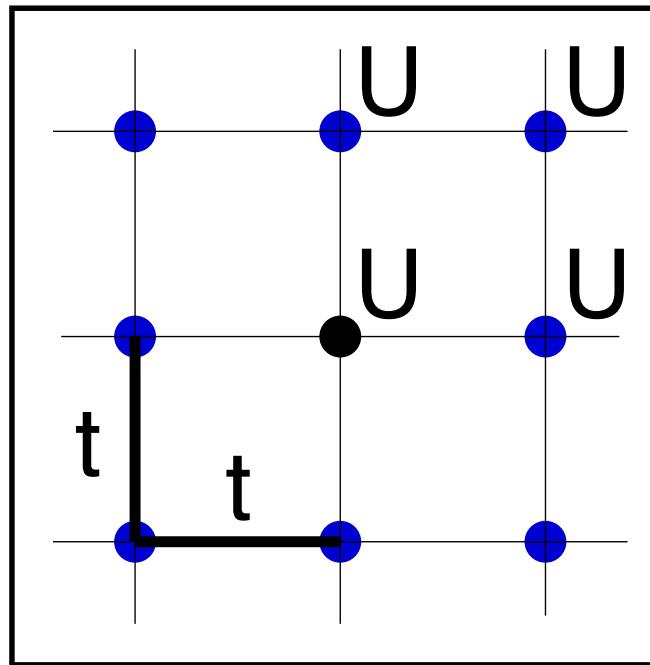
## Milestones

- dynamical mean-field theory
- topological band theory

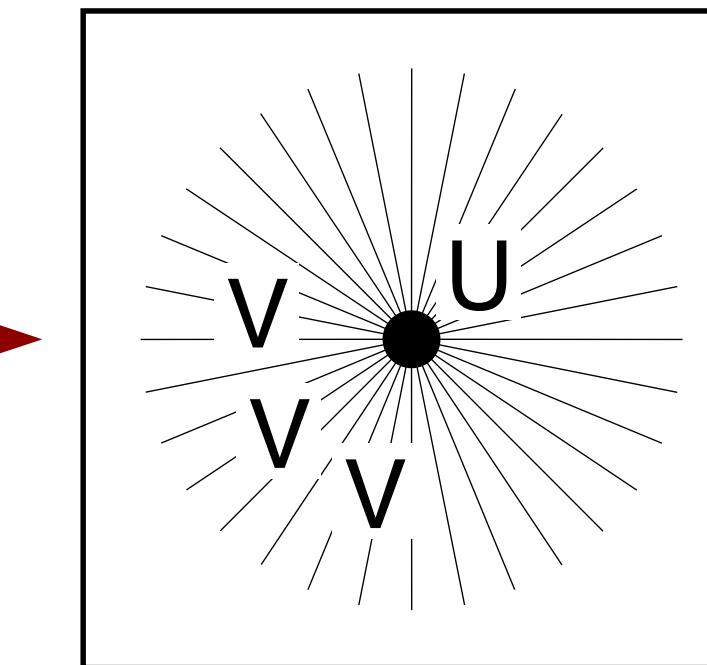
$$\text{torus } \mathbb{T}^2 \not\cong \text{circle } \mathbb{S}^1 \cong \text{cube } \mathbb{C}^2 \not\cong \text{plane}$$

# Dynamical Mean-Field Theory

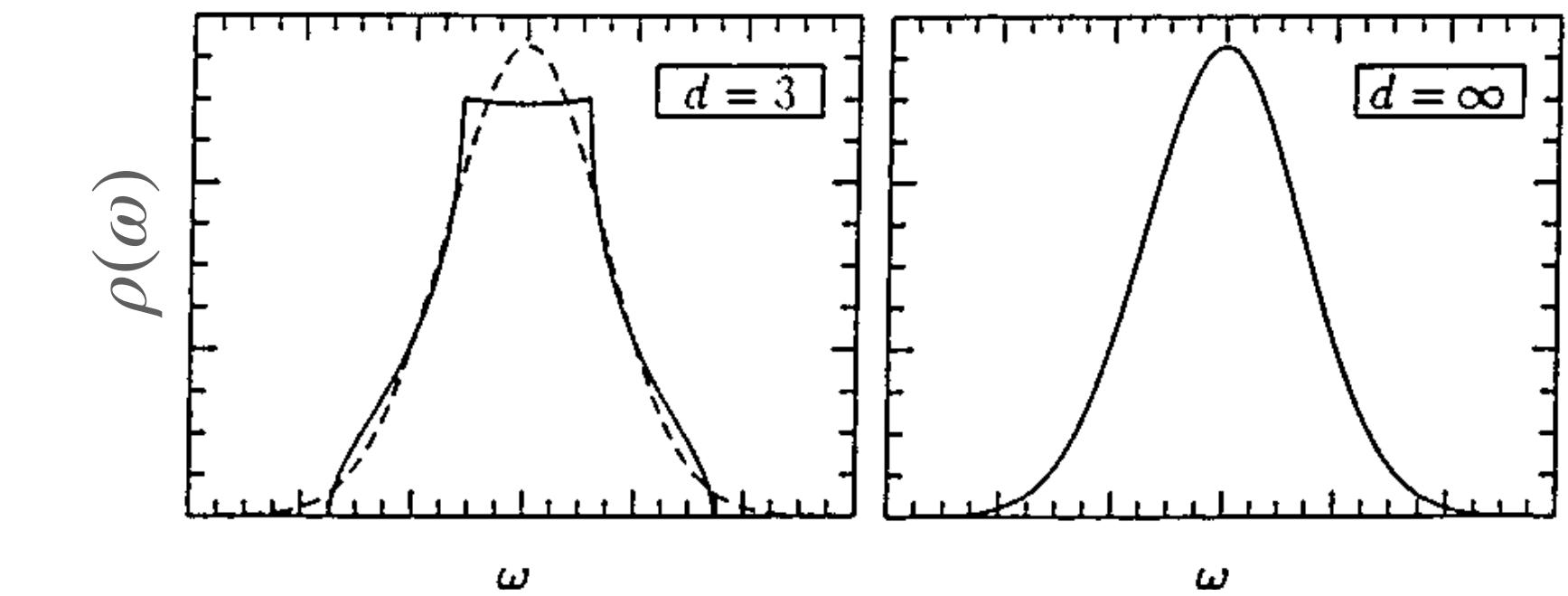
lattice fermion model



single-site impurity model



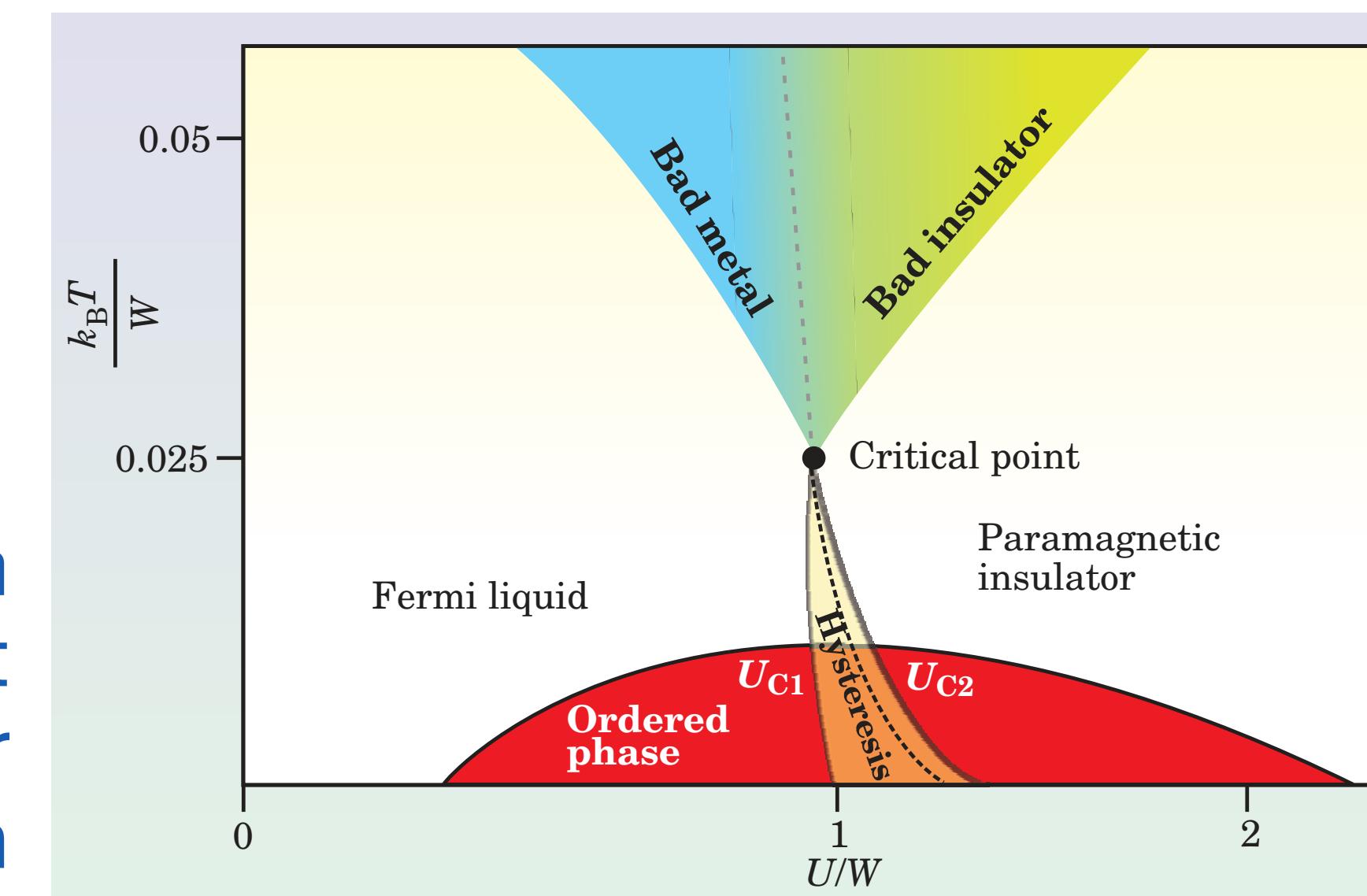
limit of infinite spatial dimensions



local electron self-energy

$$\Sigma_{ij}(\omega) = \delta_{ij}\Sigma_i(\omega)$$

phase diagram  
of the Mott  
metal-insulator  
transition



scaling of the hopping

$$t = t^*/\sqrt{D} \quad t^* = 1$$

Metzner, Vollhardt, PRL (1989)  
Müller-Hartmann, ZPB (1989)  
Georges, Kotliar, PRB (1992)  
Jarrell, PRL (1992)  
Georges, Kotliar, Krauth, Rozenberg, RMP (1996)  
Kotliar, Vollhardt, Phys. Today (2004)

# Topological Band Theory

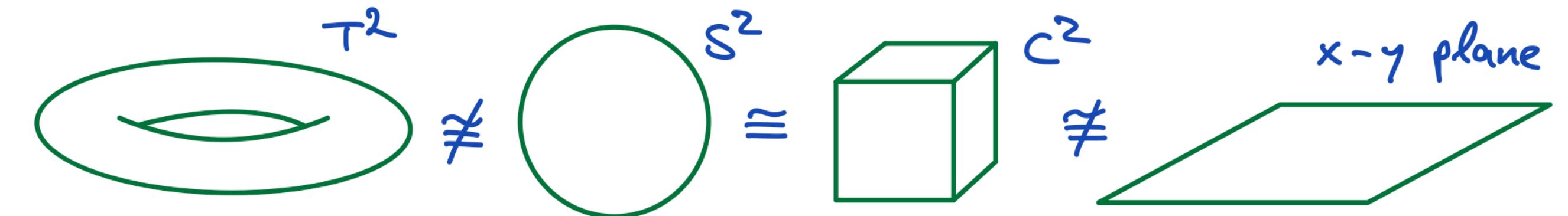
Dyson, J. Math. Phys. N.Y. (1962)

Altland, Zirnbauer, PRB (1997)

Qi, Hughes, Zhang, PRB (2008)

Schnyder, Ryu, Furusaki, Ludwig, PRB (2008)

Kitaev, AIP Conf. Proc. (2009)



Cartan \d	0	1	2	3	4	5	6	7	8
Complex case:									
A	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$ ...
AIII	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0 ...
Real case:									
AI	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$ ...
BDI	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$ ...
D	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$ ...
DIII	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0 ...
AII	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$ ...
CII	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0 ...
C	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0 ...
CI	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0 ...

Ludwig, Phys. Scr. (2016)

class A:

Chern number

$$C_D = \frac{1}{(D/2)!} \frac{i^{D/2}}{(2\pi)^{D/2}} \int_{1\text{BZ}_D} \text{tr } F^{D/2}$$

$$F = dA + A^2$$

$$A_{\alpha\beta}(k) = \langle u_\alpha(k) | \partial_k | u_\beta(k) \rangle dk$$

wrapping number:

$$T^2 = 1\text{BZ} \ni k \mapsto d(k) \in S^2$$

$$\epsilon(k) = d(k) \cdot \tau$$

# Correlations and Topology

- cluster extensions of DMFT
- nonlocal interactions and EDMFT
- two-particle level: DGammaA, DF, DB
- combination with band theory DFT+DMFT
- etc.

extensions

**dynamical mean-field theory**

- topological protection by unitary symmetries
- one-dimensional correlated models
- classification of field theories
- classical magnetism, skyrmions
- etc.

extensions

**topological band theory**

combination

topological classification of interacting lattice electron models ?

# Our Goal ?

Can we topologically classify all interacting electron models ? 

Can we topologically classify all interacting lattice electron models ? 

Can we topologically classify all lattice-electron models  
with local interactions on infinite-dimensional lattices ? 

Can we topologically classify, in infinite dimensions,  
Hubbard-type lattice models derived from noninteracting prototypes  
of the tenfold way? 

Can we topologically classify at least one of the  
prototype band models of the tenfold way, plus Hubbard-U,  
on an infinite-dimensional lattice ? 

# Topological Hamiltonian

noninteracting system, M orbitals, dimension D

$$1\text{BZ} = T^D \ni k \mapsto \epsilon(k) \in GL(M, \mathbb{R})$$

equivalently classification can be based on the map

$$k \rightarrow \mathbf{G}^{(0)}(k, \omega) = \frac{1}{\omega - \epsilon(k)}$$

interacting system: classification in terms of

$$(k, \omega) \mapsto \mathbf{G}(k, \omega) = \frac{1}{\omega - \epsilon(k) - \Sigma(k, \omega)}$$

e.g. for D=2:  $N_2 = \frac{1}{24\pi^2} \int dk_0 d^2k \text{Tr}[\epsilon^{\mu\nu\rho} G \partial_\mu G^{-1} G \partial_\nu G^{-1} G \partial_\rho G^{-1}]$

smooth interpolation

$$\mathbf{G}(k, \omega, \lambda) := \frac{1 - \lambda}{\omega - \epsilon(k) - \Sigma(k, \omega)} + \frac{\lambda}{\omega - \epsilon(k) - \Sigma(k, \omega = 0)}$$

Wang, Zhang, PRX (2012)

... if the self-energy is local

Thunström, Held, arXiv (2019)

Savrasov, Haule, Kotliar, PRL (2006)

Volovik, Zh. Eksp. Teor. Fiz. (1988)  
Ishikawa and Matsuyama, ZPC (1986)

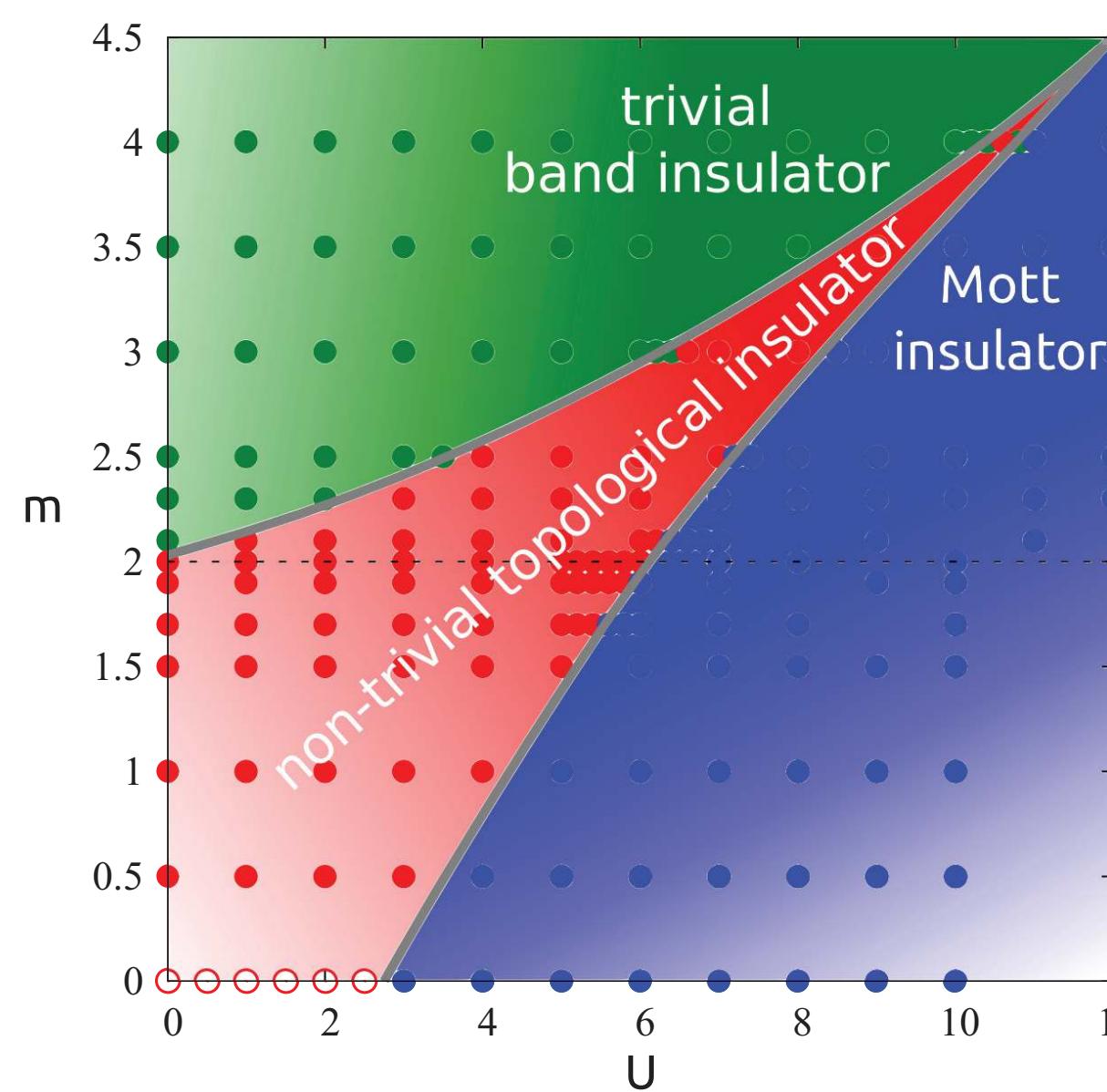
topological Hamiltonian

$$\mathbf{H}_{\text{top}}(k) = \epsilon(k) + \Sigma(\omega = 0)$$

# DMFT applied to TI's + U in D=2 or D=3

## BHZ model + U

Budich, Trauzettel, Sangiovanni, PRB (2013)

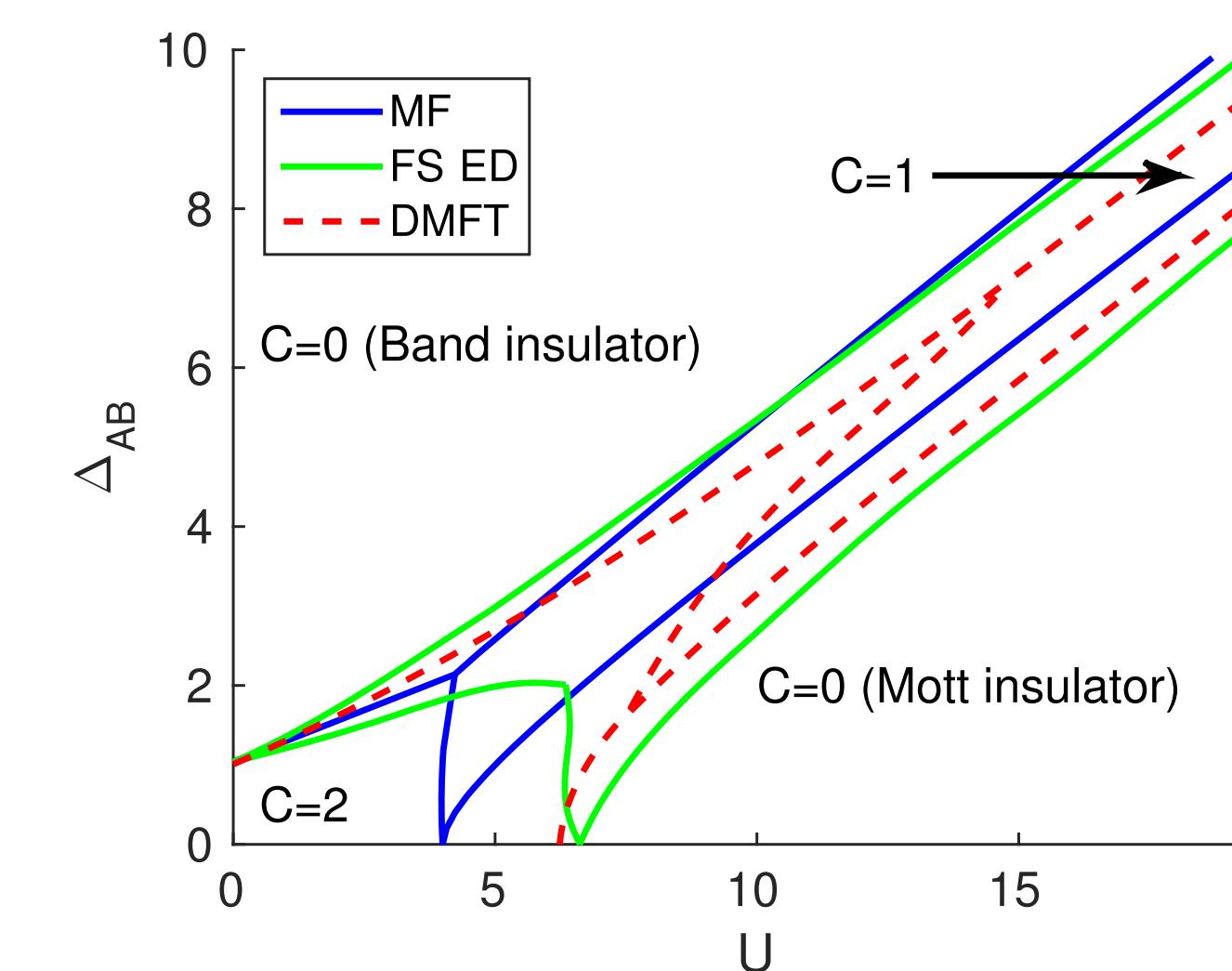


## Hofstadter butterfly + U

Markov, Rohringer, Rubtsov, PRB (2019)

## Haldane model + U

Vanhala, Siro, Liang, Troyer, Harju, Törmä , PRL (2016)

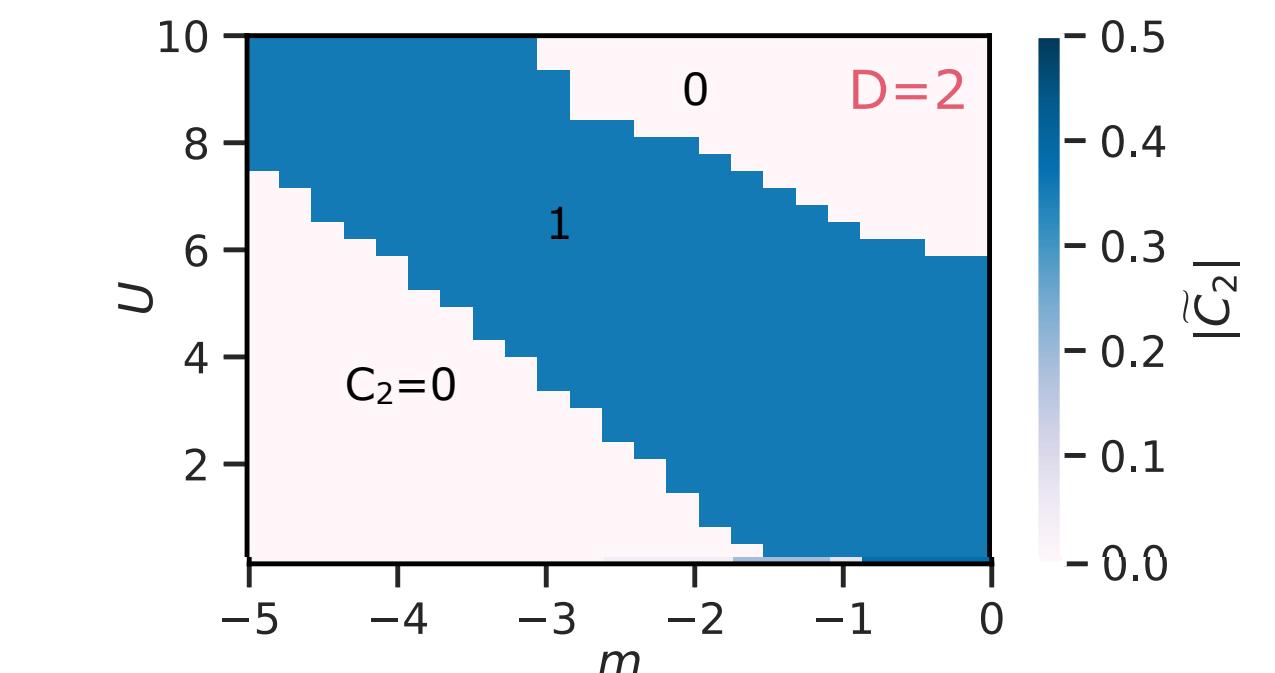


## DFT + U for SmB<sub>6</sub>

Thunström, Held, PRB (2021)

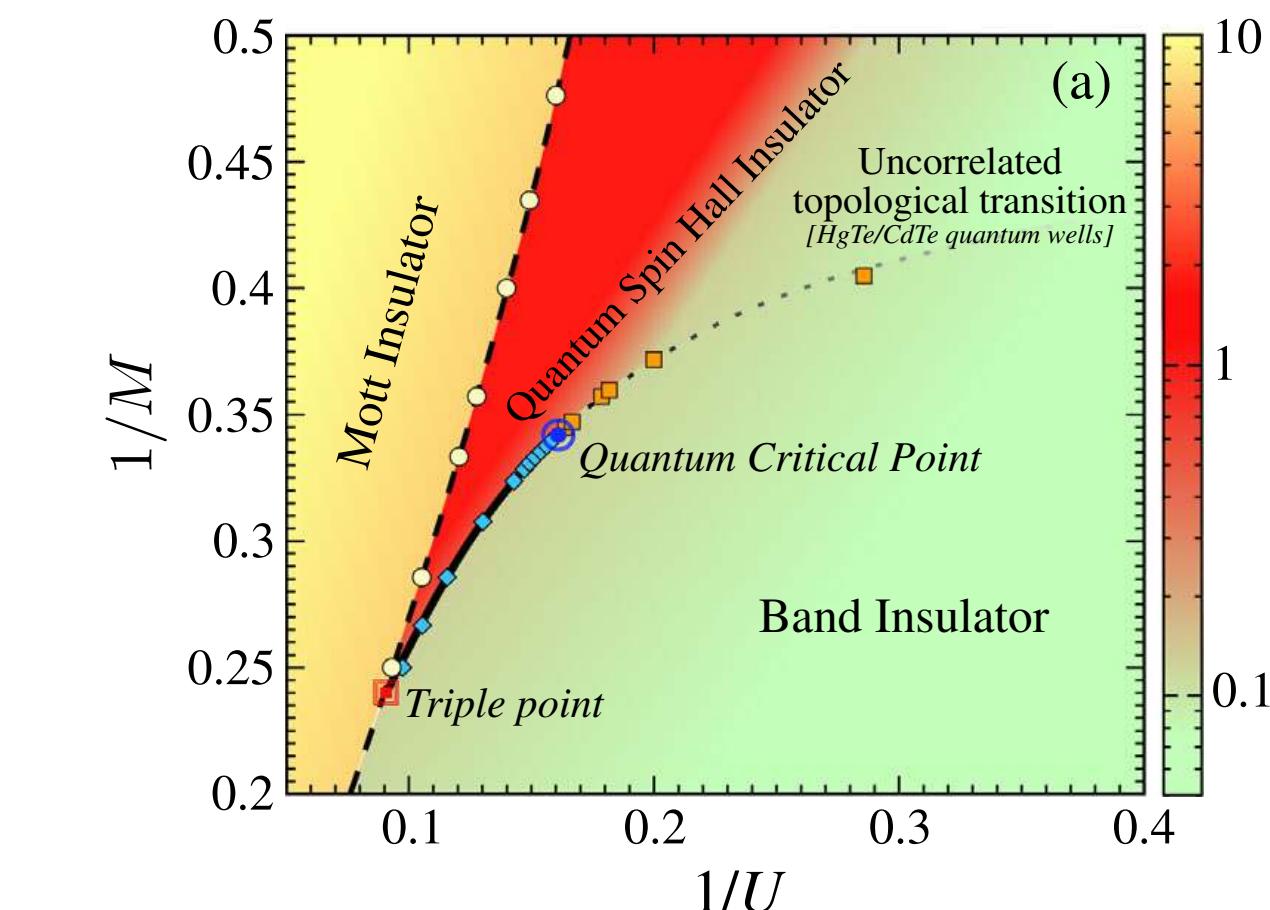
## QWZ model + U

Krüger, Potthoff, PRL (2021)



## BHZ model + U

Amaricci, Budich, Capone, Trauzettel, Sangiovanni, PRL (2015)



# Qi-Wu-Zhang (QWZ) model

D=2 square lattice, two-orbitals, broken TRS, made spinful

$$H_0 = \sum_k \sum_{\alpha, \beta=1}^M \sum_{\sigma=\uparrow, \downarrow} \epsilon_{\alpha\beta}(k) c_{k\alpha\sigma}^\dagger c_{k\beta\sigma} \quad (M=2)$$

$$\epsilon(k) = d(k) \cdot \tau \quad d(k) = \begin{pmatrix} t \sin k_x \\ t \sin k_y \\ m + t \cos k_x + t \cos k_y \end{pmatrix} \quad \tau = \begin{pmatrix} \tau_x \\ \tau_y \\ \tau_z \end{pmatrix}$$

Qi, Wu, Zhang, PRB (2006)

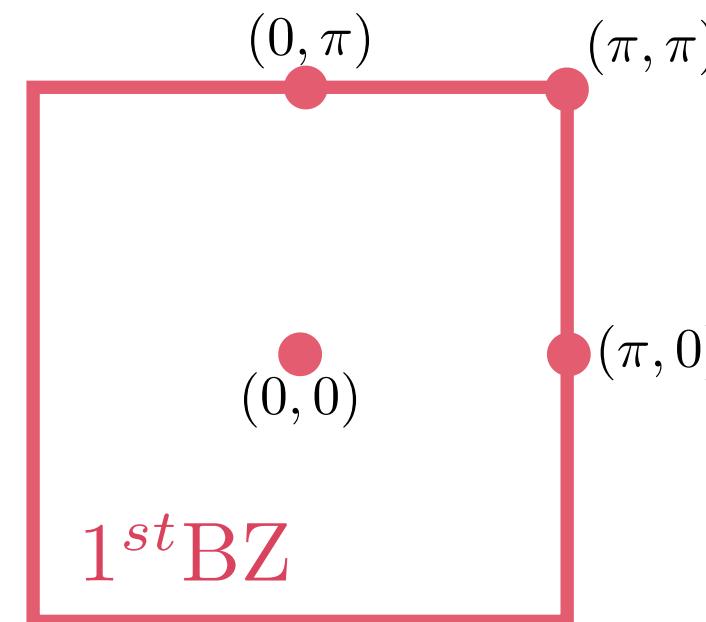
two bands:

$$\epsilon_{\pm}(k) = \pm \sqrt{t^2(\sin^2 k_x + \sin^2 k_y) + (m + t \cos k_x + t \cos k_y)^2}$$

gap closes at:

if:

- $k_x = 0, k_y = 0$  and  $m = -2t$
- $k_x = 0, k_y = \pi$  and  $m = 0$
- $k_x = \pi, k_y = 0$  and  $m = 0$
- $k_x = \pi, k_y = \pi$  and  $m = +2t$

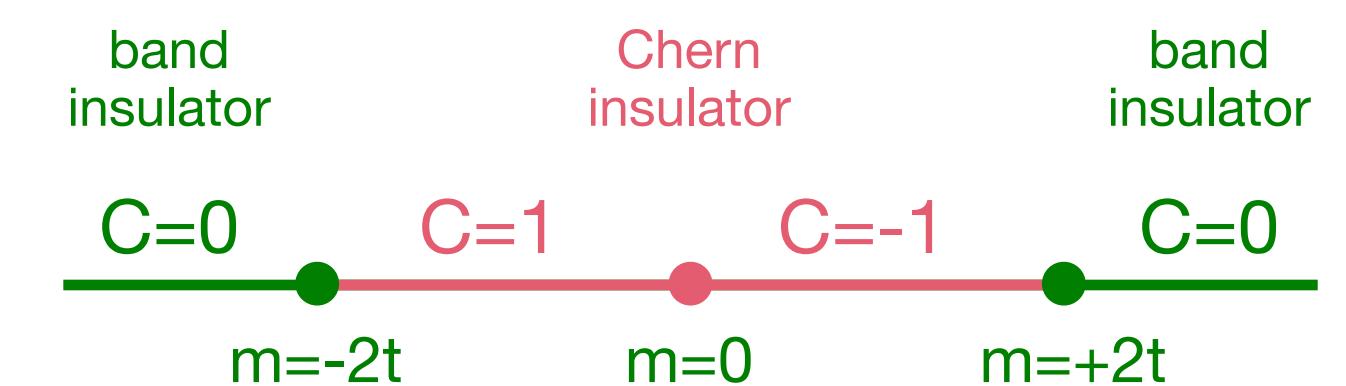


Cartan \ $d$	0	1	2	3	4	5	6	7	8
Complex case:									
A	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$ ...
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CII	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0 ...
C	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0 ...
CI	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0 ...

topological invariant:

$$C = \frac{1}{2\pi} \oint_{1\text{BZ}} d^2k F(k)$$

topological phase diagram:



# Qi-Wu-Zhang (QWZ) model

D=2 square lattice, two-orbitals, broken TRS, made spinful

$$H_0 = \sum_k \sum_{\alpha, \beta=1}^M \sum_{\sigma=\uparrow, \downarrow} \epsilon_{\alpha\beta}(k) c_{k\alpha\sigma}^\dagger c_{k\beta\sigma} \quad (M=2)$$

$$\epsilon(k) = d(k) \cdot \tau \quad d(k) = \begin{pmatrix} t \sin k_x \\ t \sin k_y \\ m + t \cos k_x + t \cos k_y \end{pmatrix} \quad \tau = \begin{pmatrix} \tau_x \\ \tau_y \\ \tau_z \end{pmatrix}$$

Qi, Wu, Zhang, PRB (2006)

can be written as (D=2)

$$\epsilon(k) = \left( m + t \sum_{r=1}^D \cos k_r \right) \gamma_D^{(0)} + t \sum_{r=1}^D \sin k_r \gamma_D^{(r)}$$

and with

$$\gamma_D^{(1)} = \tau_x \quad \gamma_D^{(2)} = \tau_y \quad \gamma_D^{(0)} = \tau_z = -i\tau_x\tau_y$$

and

$$\{\gamma_D^{(1)}, \gamma_D^{(2)}\} = \{\gamma_D^{(2)}, \gamma_D^{(0)}\} = \{\gamma_D^{(0)}, \gamma_D^{(1)}\} = 0$$

$$(\gamma_D^{(1)})^2 = (\gamma_D^{(2)})^2 = (\gamma_D^{(0)})^2 = 1$$

Cartan \ d	0	1	2	3	4	5	6	7	8
Complex case:									
A	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$ ...
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Real case:									
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C	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0 ...
CI	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0 ...

# QWZ model on the hypercubic lattice (even D)

Bloch Hamiltonian

$$\epsilon(k) = \left( m + t \sum_{r=1}^D \cos k_r \right) \gamma_D^{(0)} + t \sum_{r=1}^D \sin k_r \gamma_D^{(r)}$$

with generators of Clifford algebra

$$\begin{aligned} \{\gamma_D^{(\mu)}, \gamma_D^{(\nu)}\} &= 2\delta^{(\mu\nu)} \text{ for } \mu, \nu = 0, 1, \dots, D \\ \gamma_D^{(0)} &= (-i)^{D/2} \gamma_D^{(1)} \cdots \gamma_D^{(D)} \end{aligned}$$

band dispersions

$$\epsilon(k)^2 = \left( \sum_{\mu=0}^D d_\mu(k) \gamma_D^{(\mu)} \right)^2 = \sum_{\mu\mu'} d_\mu(k) d_{\mu'}(k) \gamma_D^{(\mu)} \gamma_D^{(\mu')} = \left( d_0(k)^2 + \sum_{r=1}^D d_r(k)^2 \right) \mathbf{1}$$

$$\epsilon(k) = \pm \left( (m + t \sum_r \cos k_r)^2 + \sum_r t^2 \sin^2 k_r \right)^{1/2}$$

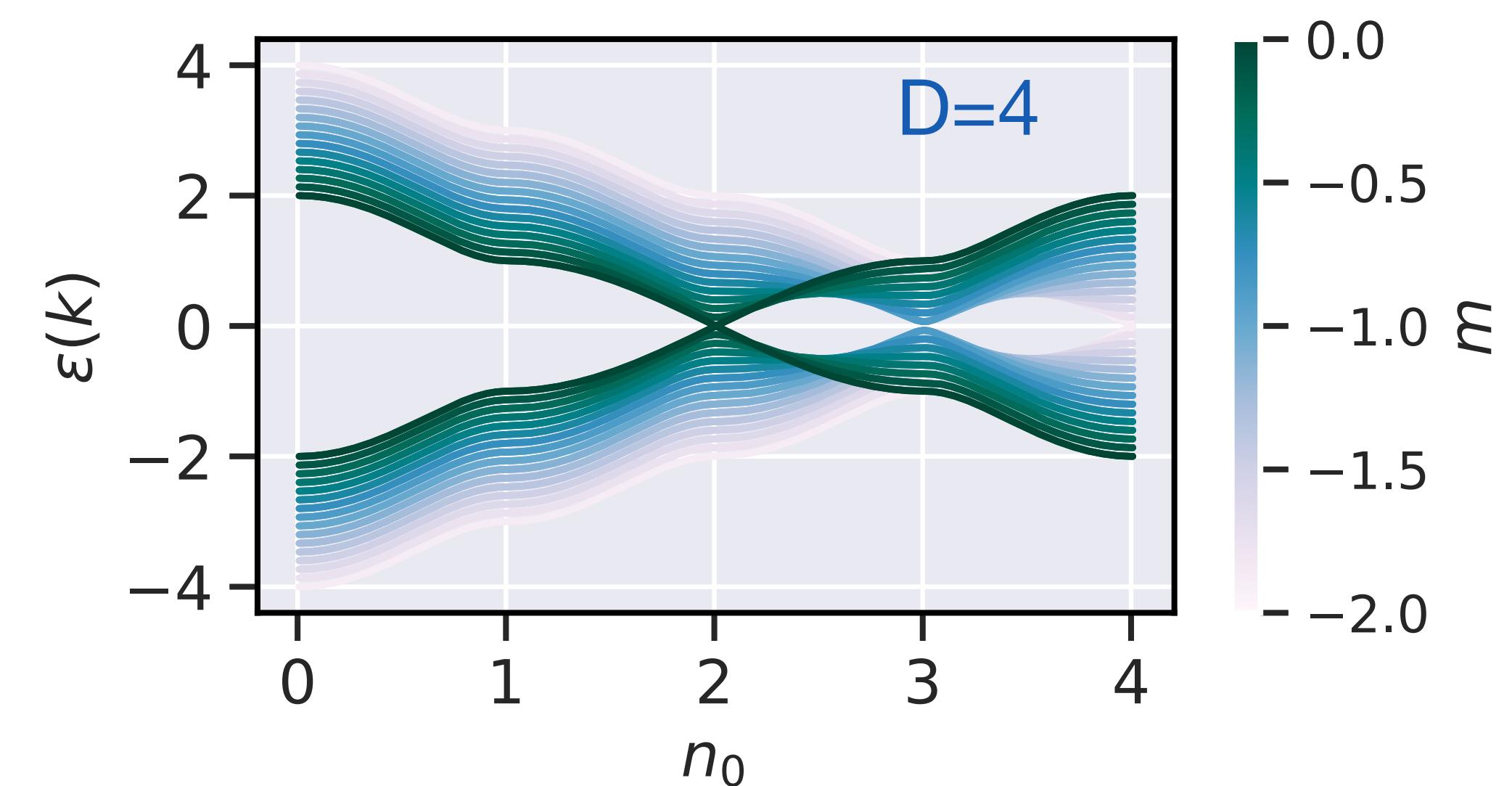
gap closure for

$$m = (D - 2n_0)t$$

at  $\binom{D}{n_0}$  HSPs

$$k_{n_0} = (\underbrace{0, \dots, 0}_{n_0}, \pi, \dots, \pi)$$

in the 1BZ



# $D \rightarrow \infty$ limit and scaling of the hopping

free Green's function of orbital  $\alpha$

$$G_{\alpha\alpha}^{(0)}(k, \omega) = \left[ \frac{\omega + \sum_\mu d_\mu(k) \gamma_D^\mu}{\omega^2 - \sum_\mu d_\mu(k)^2} \right]_{\alpha\alpha} = \sum_{n=0}^{\infty} \frac{M_\alpha^{(n)}(k)}{\omega^{n+1}}$$

$\gamma_D^{(0)} = \text{diag}(+1, -1, \dots)$

moments of the local DOS of orbital  $\alpha$

$$M_\alpha^{(0)} = 1$$

$$M_\alpha^{(1)} = m \gamma_{\alpha\alpha}^{(0)} = \pm m$$

$$M_\alpha^{(2)} = t^2 D + m^2 = t^{*2} + m^2$$

with the usual scaling

$$t = t^* / \sqrt{D} \quad t^* = 1$$

band edges

$$\epsilon_{\max, \min} = \pm(|m| + \sqrt{D}t^*) \mapsto \pm\infty$$

A and B orbitals

$$M_\alpha^{(n)} = \frac{1}{L} \sum_k M_\alpha^{(n)}(k) = \int d\omega \omega^k \rho_\alpha(\omega)$$

band closures at

$$m = \left( \sqrt{D} - 2 \frac{n_0}{\sqrt{D}} \right) t^* \quad (n_0 = 0, \dots, D)$$

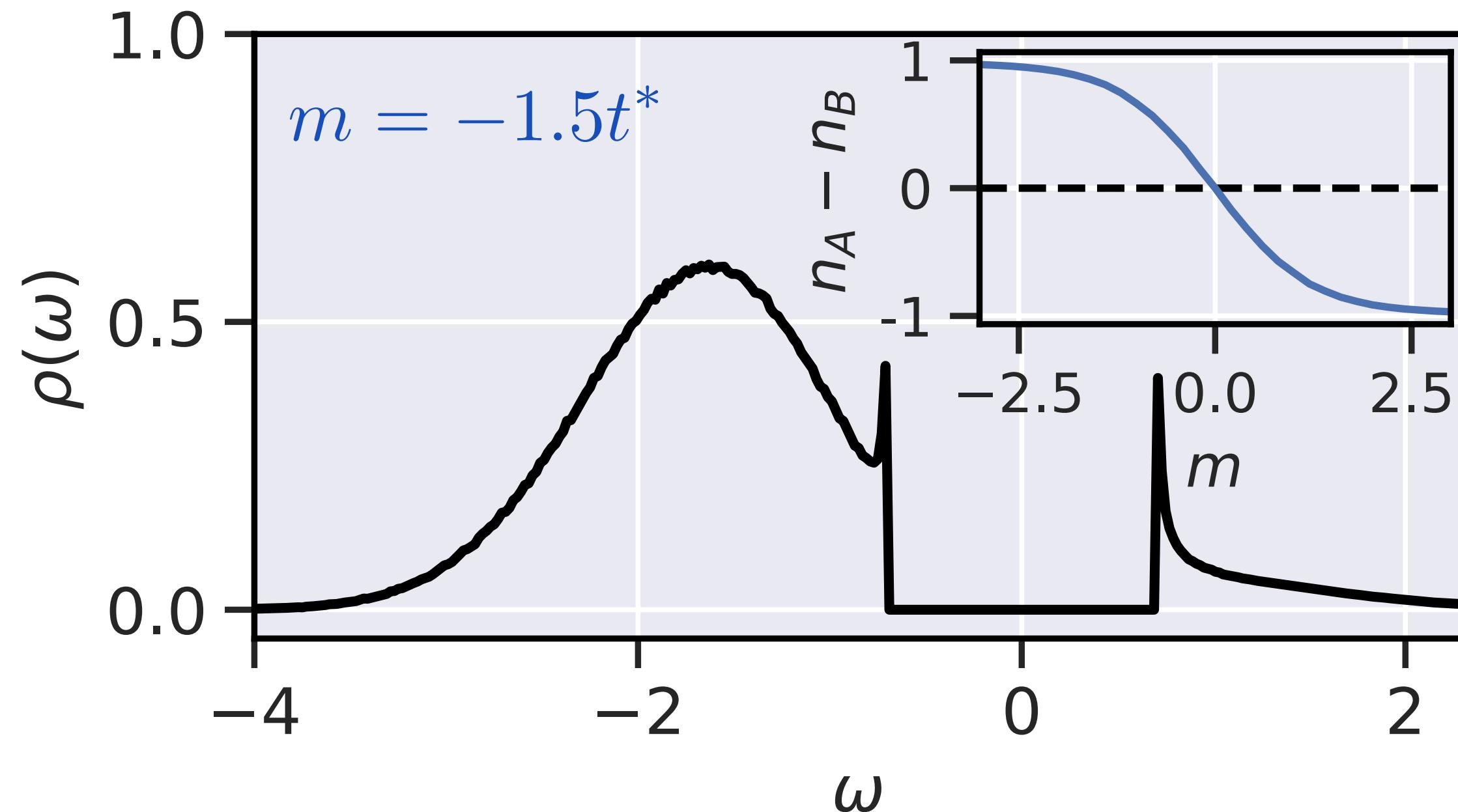
$$D = 2 : \quad m = \sqrt{2}t^*, 0, -\sqrt{2}t^*$$

$$D = 4 : \quad m = -2t^*, -t^*, 0, t^*, 2t^*$$

$$D = 6 : \quad m = \sqrt{6}t^*, \frac{2}{3}\sqrt{6}t^*, \frac{1}{3}\sqrt{6}t^*, 0, -\frac{1}{3}\sqrt{6}t^*, -\frac{2}{3}\sqrt{6}t^*, -\sqrt{6}t^*$$

:

# DOS in the $D \rightarrow \infty$ limit



local DOS of orbital  $\alpha$  in the limit  $D \rightarrow \infty$

$$\rho_\alpha(\omega) = \frac{1}{2} \frac{1}{t^* \sqrt{\pi}} \Theta(|\omega| - \frac{1}{\sqrt{2}} t^*) \text{sign } \omega \sum_{s=\pm} \left( \frac{\omega}{\sqrt{\omega^2 - \frac{1}{2} t^{*2}}} + sz_\alpha \right) \exp \left( - \frac{\left( s \sqrt{\omega^2 - \frac{1}{2} t^{*2}} - m \right)^2}{t^{*2}} \right)$$

there is a finite gap  $\Delta = \sqrt{2}t^*$  independent of  $m$ !

# Irreps of Clifford algebra

Bloch Hamiltonian

$$\epsilon(k) = \left( m + t \sum_{r=1}^D \cos k_r \right) \gamma_D^{(0)} + t \sum_{r=1}^D \sin k_r \gamma_D^{(r)}$$

with generators of Clifford algebra

$$\{\gamma_D^{(\mu)}, \gamma_D^{(\nu)}\} = 2\delta^{(\mu\nu)} \text{ for } \mu, \nu = 0, 1, \dots, D$$

Theorem

- for even D, there is a **unique** irrep of the complex Clifford algebra
- $\mathbb{C}l_{D+2} \cong \text{Mat}(2, \mathbb{C}) \otimes \mathbb{C}l_D$
- dimension of the representation:  $M = 2^{D/2}$

explicit iterative construction

$$\begin{aligned}\gamma_{D+2}^{(r)} &= \tau_x \otimes \gamma_D^{(r)}, \text{ for } r = 1, \dots, D \\ \gamma_{D+2}^{(D+1)} &= \tau_x \otimes \gamma_D^{(0)}, \quad \gamma_{D+2}^{(D+2)} = \tau_y \otimes \mathbf{1} \\ \gamma_{D+2}^{(0)} &= \tau_z \otimes \mathbf{1}.\end{aligned}$$

Prodan, Schulz-Baldes (2016)  
“Bulk and Boundary Invariant for Complex Topological Insulators”

immediate consequences

- number of orbitals  $M = 2^{D/2}$  (diverges for  $D \rightarrow \infty$ )
- A- and B-orbitals ( $m$ : strength of staggered orbital field)
- degenerate band structure

# Chern number

$$C_D = \frac{1}{(D/2)!} \frac{i^{D/2}}{(2\pi)^{D/2}} \int_{1BZ_D} \text{tr } F^{D/2}$$

$$F = dA + A^2$$

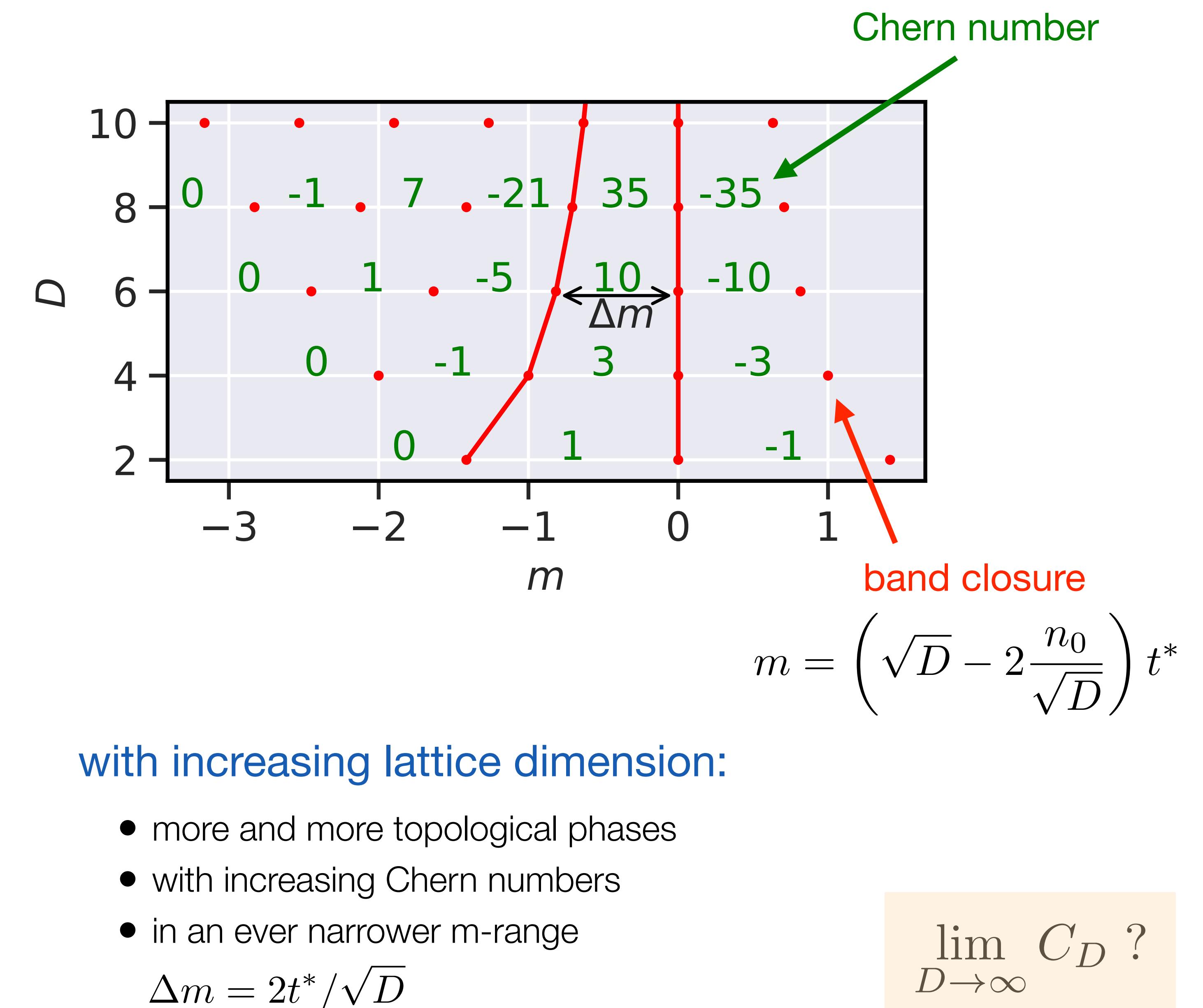
$$A_{\alpha\beta}(k) = \langle u_\alpha(k) | \partial_k | u_\beta(k) \rangle dk$$

K-theory yields: Prodan, Schulz-Baldes (2016)

$$C_D(n_0) = (-1)^{n_0 + \frac{D}{2}} \binom{D-1}{n_0}$$

## interpretation

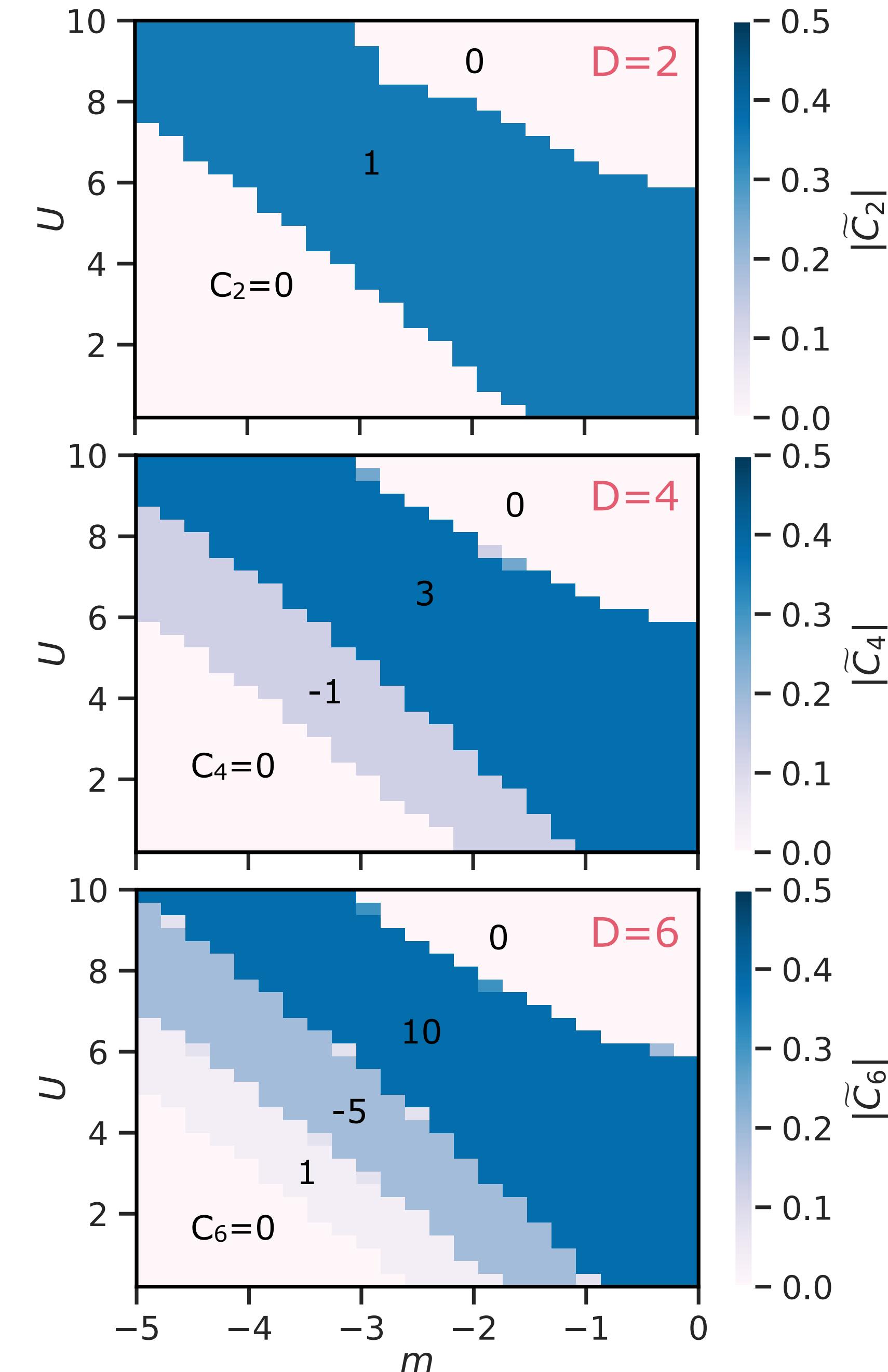
- (D-1)-dim. (1000...) surface hosts  $\binom{D-1}{n_0}$  gapless edge states
- Weyl nodes at surface-projected HSP's  $k_{n_0}$  in the (D-1)-dim surface BZ
- sign: chirality of the Weyl points



# DMFT of QWZ+U

topological phase diagrams  
for even finite D at half-filling

- trivial band insulator, trivial Mott insulator
- nontrivial intermediate phases
- more phases with increasing D
- phase diagram symmetric  $m \leftrightarrow -m$
- at  $m=0$ : transition from an interacting Chern insulator to trivial Mott insulator
- strong A-B orbital polarization:  
 $\Sigma_A \rightarrow U, \Sigma_B \rightarrow 0$  for  $m \rightarrow \infty$
- $U_c(m) \sim |m|$  for  $m \rightarrow \pm \infty$



topological  
Hamiltonian

$$\mu \rightarrow \mu + \Sigma_+(\omega = 0)$$

$$m \rightarrow m + \Sigma_-(\omega = 0)$$

$$\Sigma_{\pm} = \frac{1}{2}(\Sigma_A \pm \Sigma_B)$$

# Chern density

Chern number

$$C_D(n_0) = (-1)^{n_0 + \frac{D}{2}} \binom{D-1}{n_0}$$

sum rule

$$\sum_{n_0=0}^{D-1} \frac{1}{2^{D-1}} |C_D(n_0)| = 1$$

define:

$$c(n_0) = \frac{1}{2^{D-1}} \binom{D-1}{n_0} \xrightarrow{D \rightarrow \infty} \sqrt{\frac{2}{\pi D}} \exp\left(-2 \frac{[(D/2) - n_0]^2}{D}\right)$$

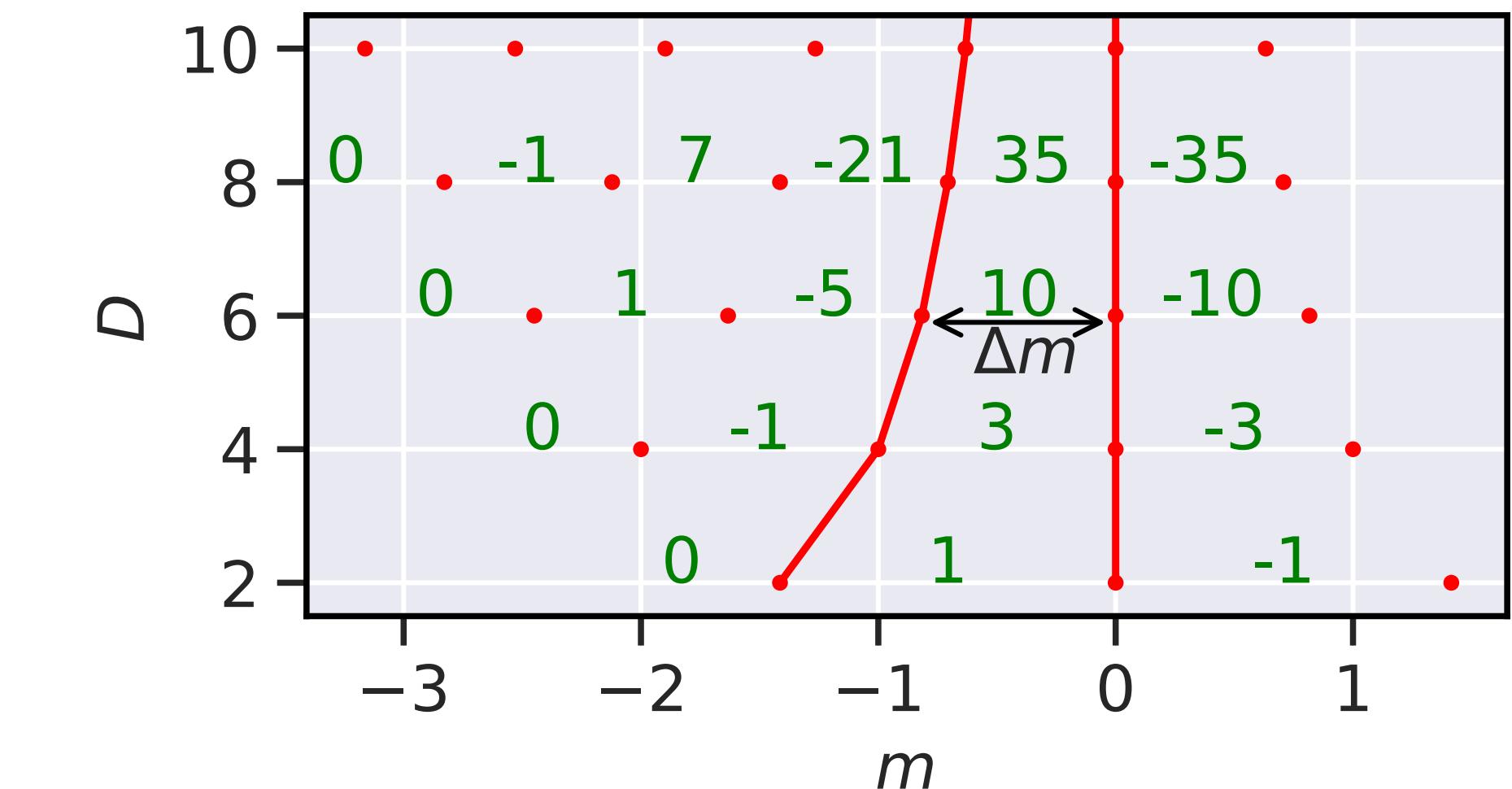
$$= \sqrt{\frac{2}{\pi D}} \exp\left(-\frac{1}{2} \frac{m^2}{t^{*2}}\right) = \underbrace{\frac{2t^*}{\sqrt{D}}}_{\text{continuum limit}} \frac{1}{t^* \sqrt{2\pi}} \exp\left(-\frac{1}{2} \frac{m^2}{t^{*2}}\right) \equiv c(m) dm$$

band closure condition

$$m = \left(\sqrt{D} - 2 \frac{n_0}{\sqrt{D}}\right) t^*$$

every m is critical !

$$\Delta m = 2t^*/\sqrt{D} \rightarrow dm$$

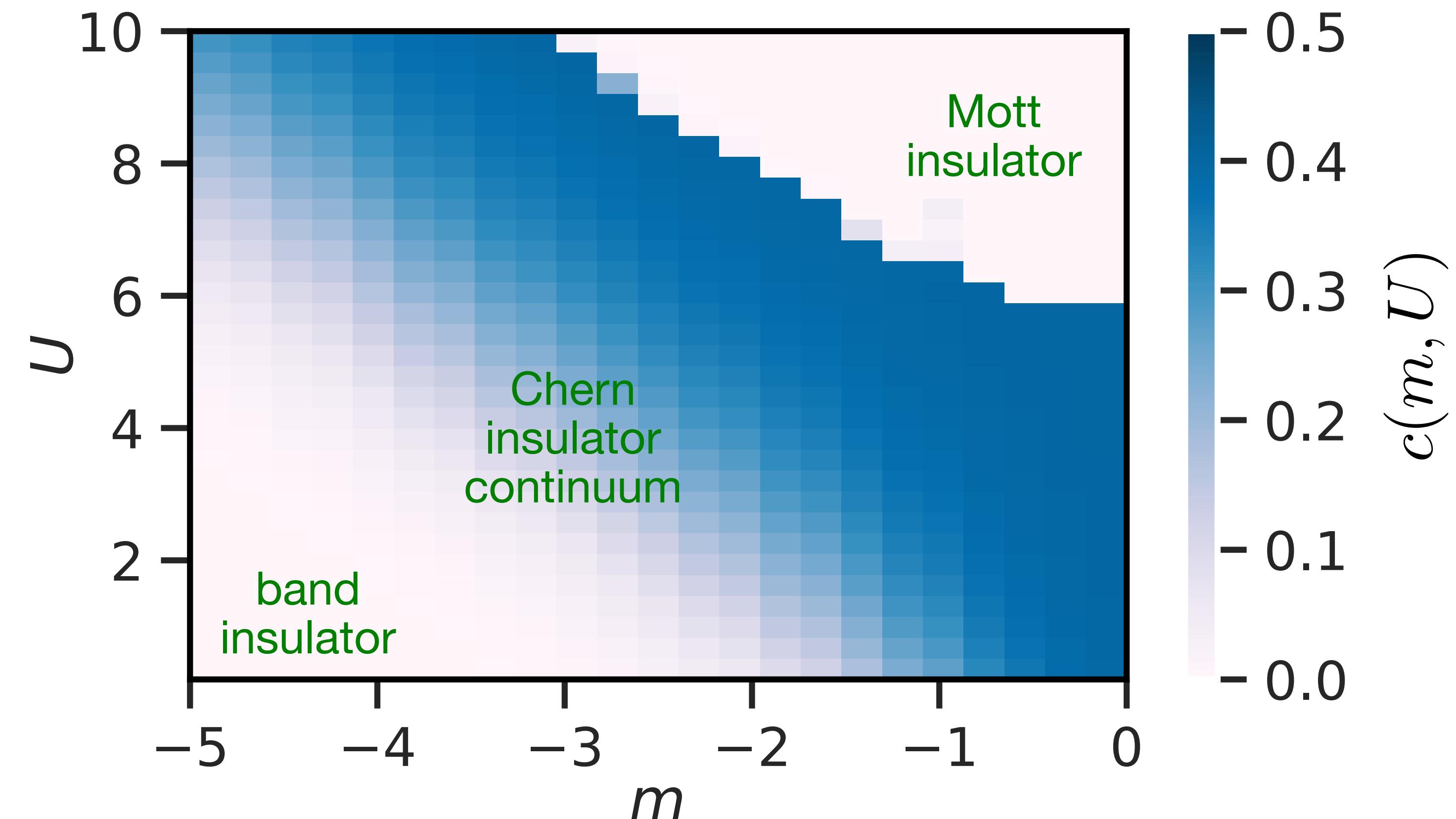


Chern density

$$c(m) = \frac{1}{t^* \sqrt{2\pi}} e^{-\frac{1}{2} \frac{m^2}{t^{*2}}}$$

$$\int_{-\infty}^{\infty} c(m) dm = 1$$

# Phase diagram of the $D \rightarrow \infty$ QWZ+U model



- on iso-Chern lines: topologically equivalent systems
- continuum of topologically different phases on paths crossing iso-Cherns

# Electronic structure

for  $m = \left( \sqrt{D} - 2 \frac{n_0}{\sqrt{D}} \right) t^*$  the Bloch Hamiltonian

$$\epsilon(k) = \left( m + t \sum_{r=1}^D \cos k_r \right) \gamma_D^{(0)} + t \sum_{r=1}^D \sin k_r \gamma_D^{(r)}$$

close to one of the  $\binom{D}{n_0}$  equivalent HSPs  $k_{n_0} = (\underbrace{0, \dots, 0}_{n_0}, \pi, \dots, \pi)$  in the 1BZ

leads to a Dirac-cone dispersion

$$\epsilon_{\pm}(k) = \pm \frac{t^*}{\sqrt{D}} \sqrt{\sum_{r=1}^D (k_r - k_{n_0, r})^2}$$

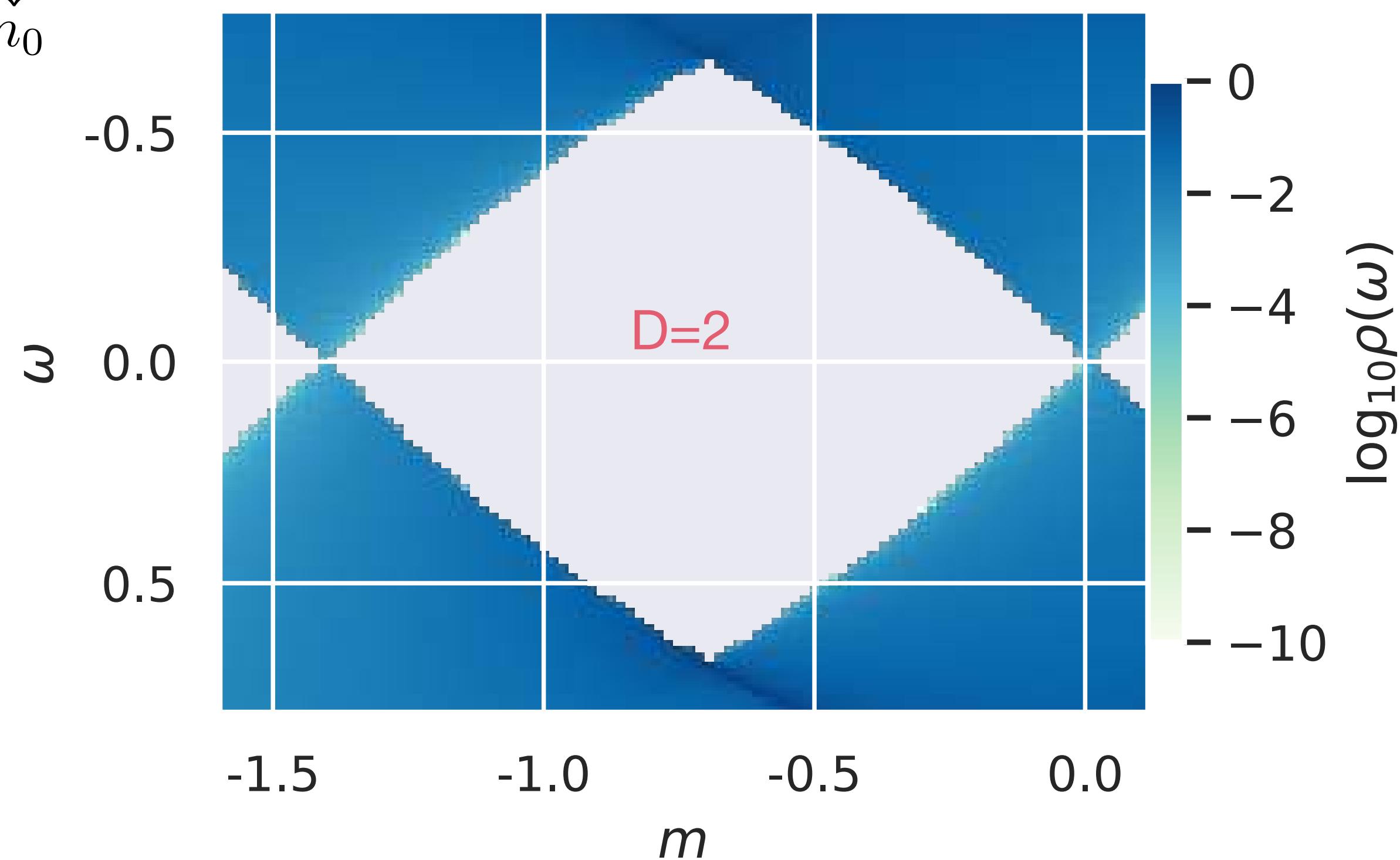
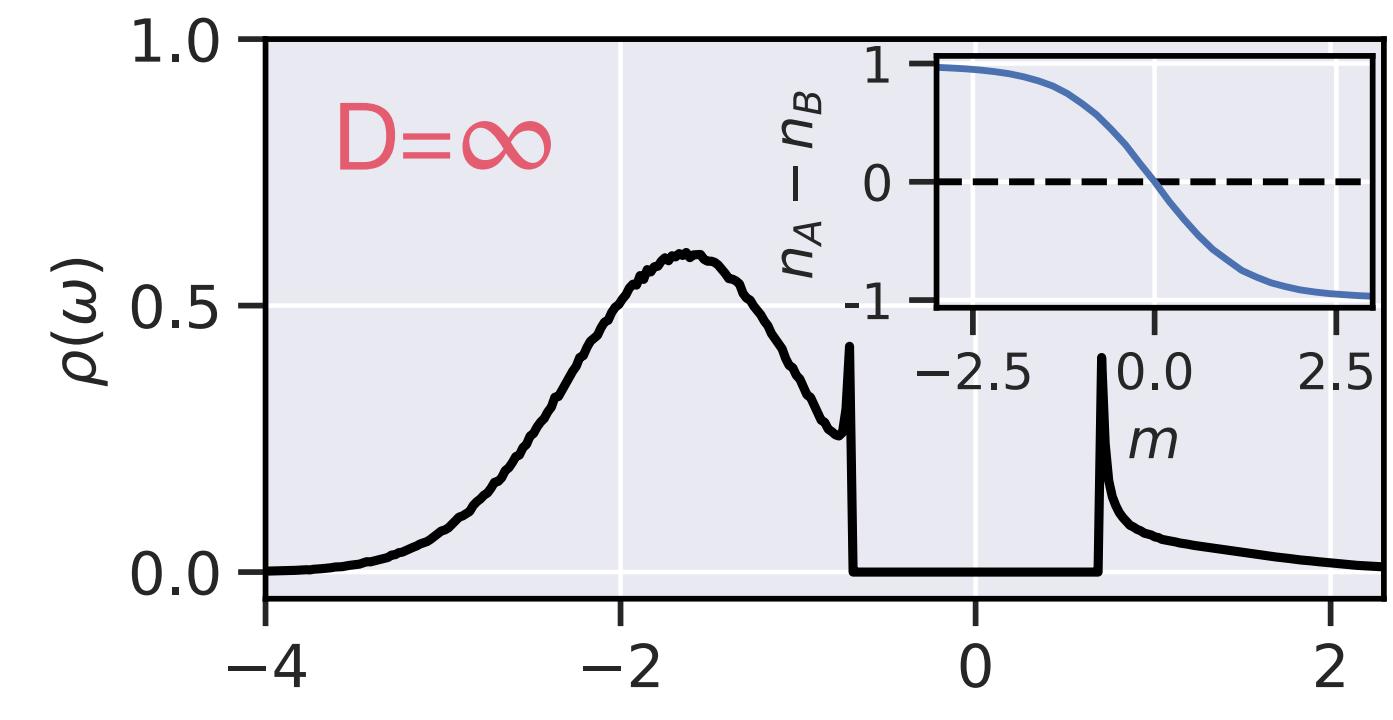
local DOS at low frequencies

$$\rho_{\alpha}(\omega) = c(D, n_0) |\omega|^{D-1} / t^{*D}$$



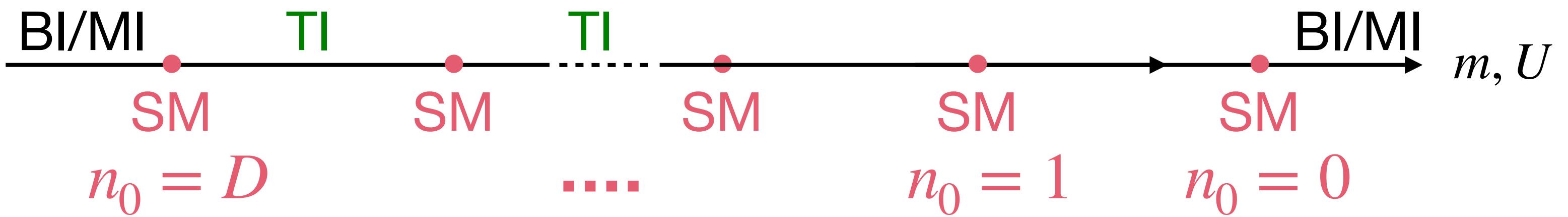
$c(D, n_0) \rightarrow 0$  for  $D \rightarrow \infty$  exponentially fast

$$\Delta = \sqrt{2}t^*$$



# Semimetal vs. topological insulator

finite dimension D:



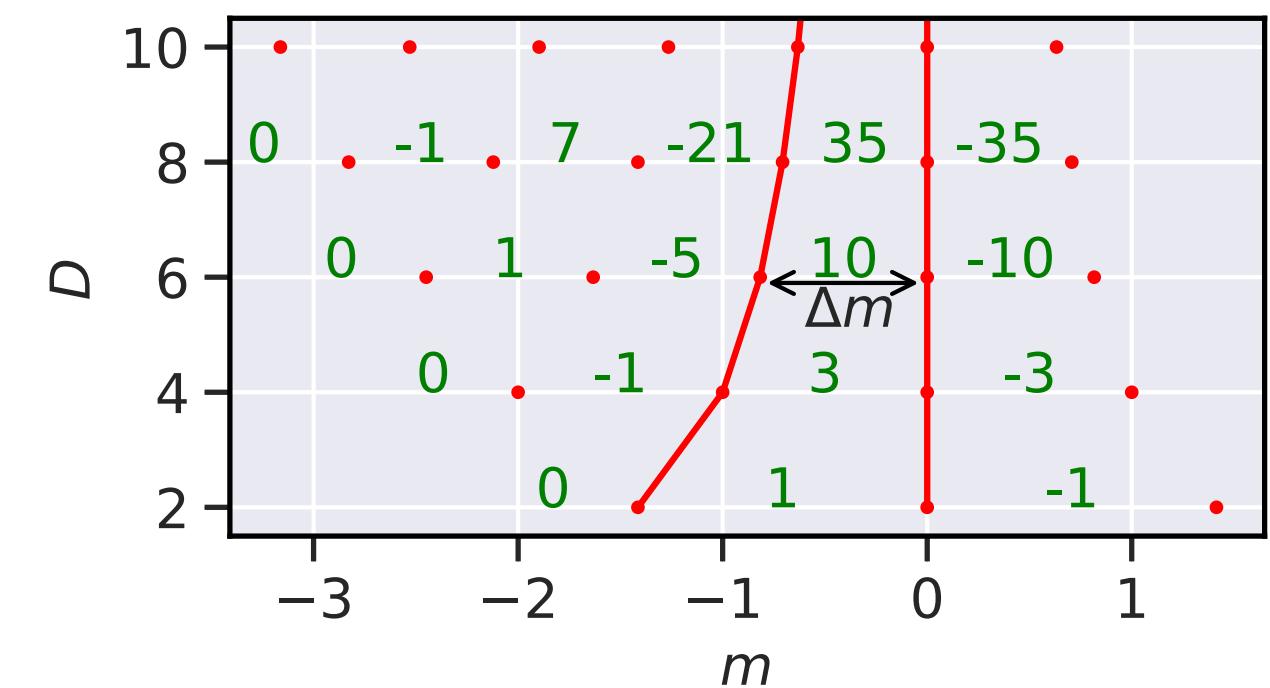
infinite dimensions:

- Chern density  $c(m, U)$  varies continuously     $\Delta m = 2t^*/\sqrt{D} \rightarrow dm$
- distinction between SM and TI not meaningful
- there is no “band closure at isolated k-points in the 1BZ”

$$\text{Dirac cone: } \epsilon_{\pm}(k) = \pm t^* \sqrt{\frac{1}{D} \sum_{r=1}^D (k_r - k_{n_0, r})^2} = \pm t^* \|k - k_{n_0}\|$$

$$\text{here } \|k\|^2 = \lim_{D \rightarrow \infty} \frac{1}{D} \sum_{r=1}^D k_r^2$$

$$\text{but } \|k\| = 0 \not\Rightarrow k = 0 \quad \|\cdot\| \text{ is a semi-norm}$$



$$m = \left( \sqrt{D} - 2 \frac{n_0}{\sqrt{D}} \right) t^*$$

$$k_{n_0} = (\underbrace{0, \dots, 0}_{n_0}, \pi, \dots, \pi)$$

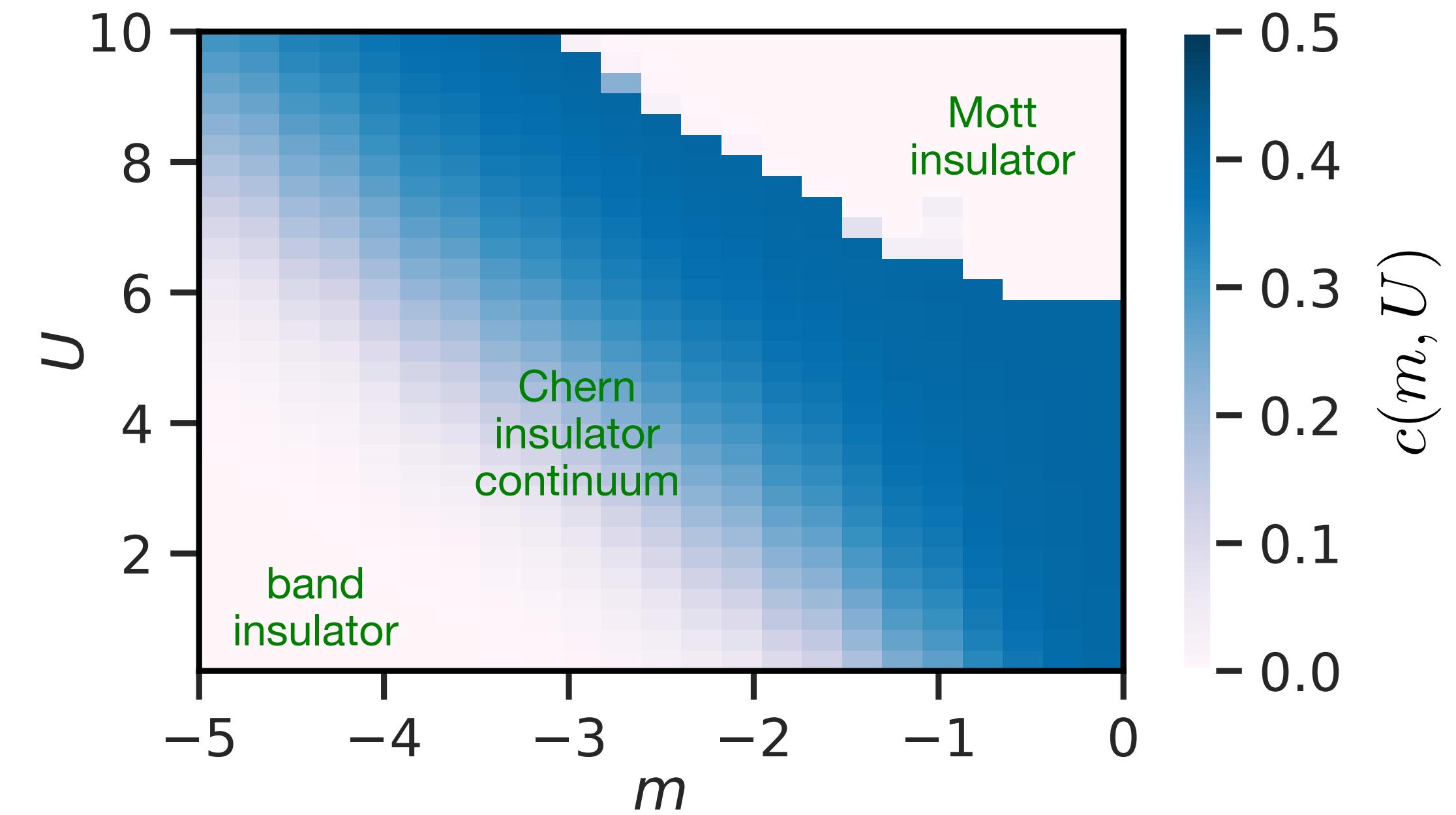
# Conclusions

## What survives $D \rightarrow \infty$ ?

- local correlations effects
- nontrivial topological classification
- the overall structure of the finite-D phase diagrams
- DMFT solves the problem exactly

## What does not ?

- distinction between semi-metal / insulator states
- arguments based on the discreteness of the topological invariant
- Chern density is positive: chirality of edge modes ?
- there is not  $the D \rightarrow \infty$  limit (only even D considered)



D. Krüger, M.P., PRL (2021)

# To do

Can we topologically classify all interacting electron models ? 

Can we topologically classify all interacting lattice electron models ? 

Can we topologically classify all lattice-electron models  
with local interactions on infinite-dimensional lattices ? 

Can we topologically classify, in infinite dimensions,  
Hubbard-type lattice models derived from noninteracting prototypes  
of the tenfold way? 

Can we topologically classify at least one of the  
prototype band models of the tenfold way, plus Hubbard-U,  
on an infinite-dimensional lattice ? 