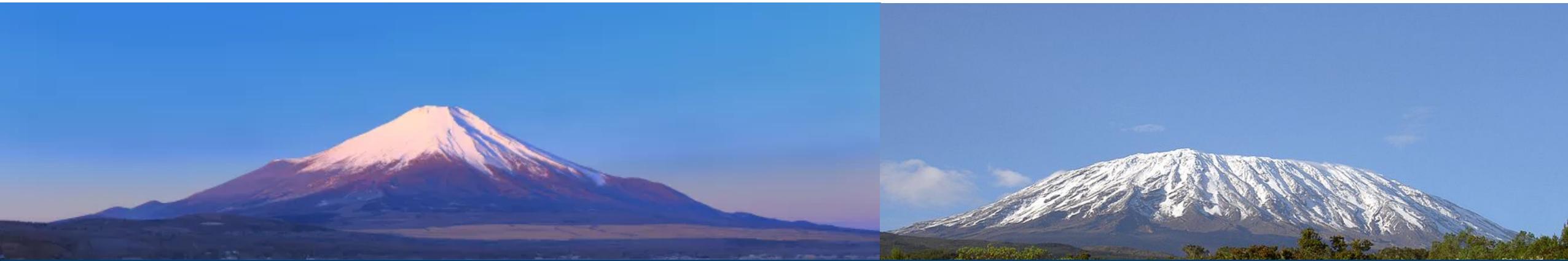


EFFECTIVE (FIELD) THEORIES FOR LOW-DIMENSIONAL SYSTEMS

JUNE 5, 2024, CLOSING MEETING

CRC110 “SYMMETRIES AND THE EMERGENCE OF STRUCTURE IN QCD”

THOMAS LUU, IAS-4/FZJ



EFFECTIVE (FIELD) THEORIES FOR LOW-DIMENSIONAL SYSTEMS

JUNE 5, 2024, CLOSING MEETING

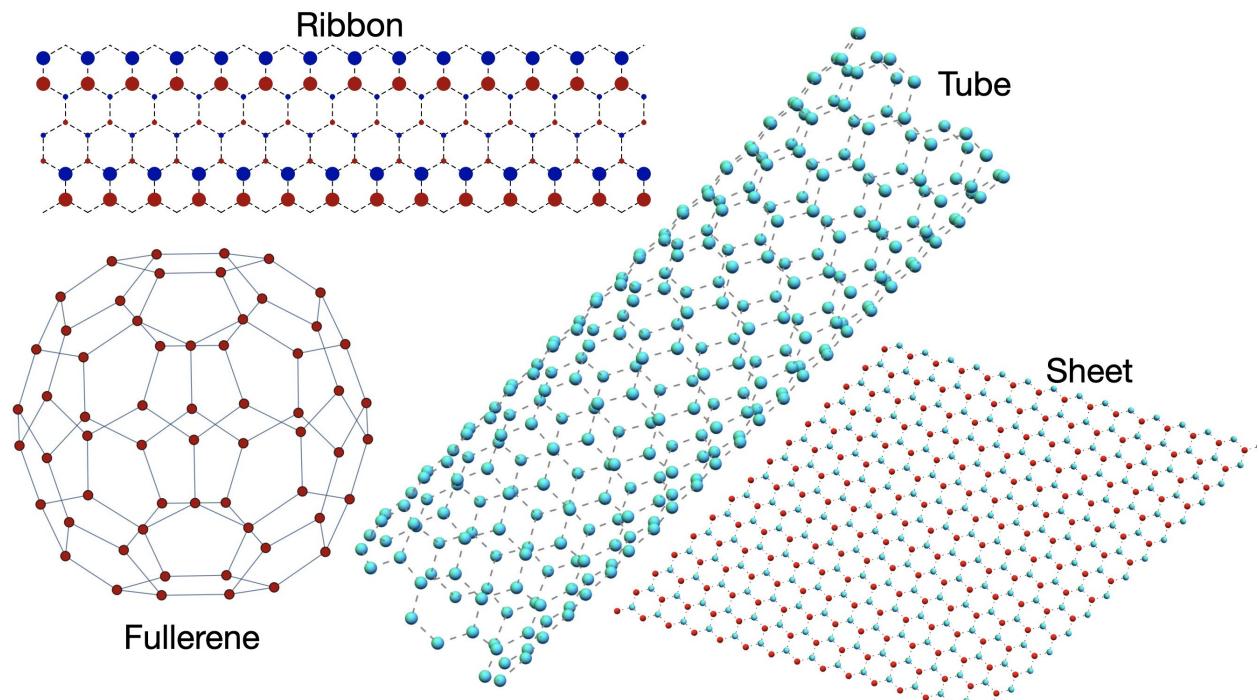
CRC110 “SYMMETRIES AND THE EMERGENCE OF STRUCTURE IN QCD”

THOMAS LUU, IAS-4/FZJ



WHY LOW-D MATERIALS?

- At least one of the dimensions of the material is small (~ nanoscale)
- Quantum effects and strong correlations induce novel phenomena
- Novel quantum electronics
- Fault tolerant quantum computing



WHY DO WE EXPECT STRONG CORRELATIONS IN LOW -D?

Isn't QED perturbative?

Let's first assume a quadratic dispersion relation:

$$E_k \approx n_d^{2/d} (2m^*) \quad : \quad n_d = 1/l^d$$

Average kinetic energy of electron Density of electrons Effective mass Mean distance between electrons Dimension of system

$$E_C \approx e^2 n_d^{1/d} / \epsilon_0 \quad : \quad V(r) = \frac{e^2}{\epsilon_0 r}$$

Average Coulomb energy of electron Dielectric constant (depends on medium)

$$\Gamma = \frac{E_C}{E_K} \propto (n_0/n_d)^{1/d} \quad : \quad n_0 = (m^* e^2 / \epsilon_0)^d$$

Fiducial density

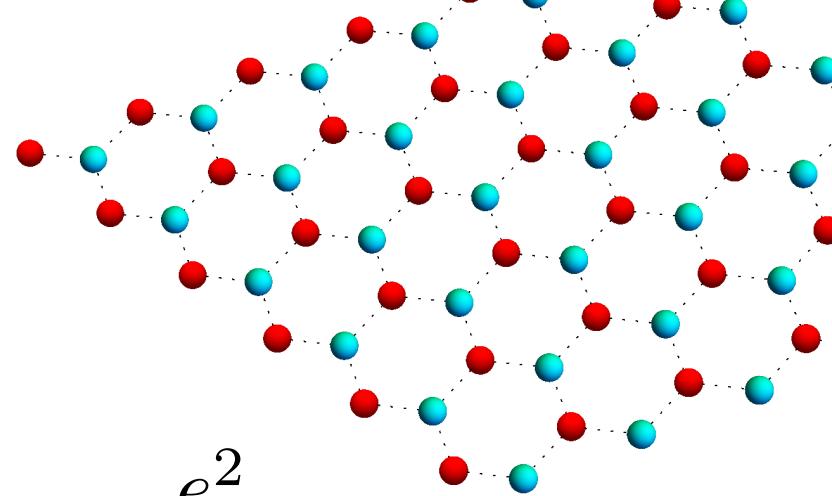
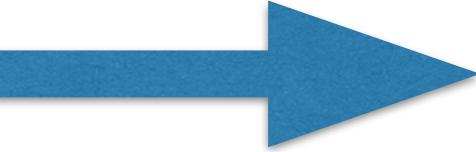
Strength of electron correlations depends on density of electrons and dimensionality of system

2D EXAMPLE: GRAPHENE

Honeycomb lattice

Use linear dispersion and set d = 2:

$$E_K \approx v_F n^{1/2}$$



$$\Gamma = \frac{e^2}{\epsilon_0 v_F}$$

Independent of electron density!

Let's plug in some numbers:

$$v_F \approx \frac{c}{300} \rightarrow \Gamma \approx 2 - 3$$

The electrons in graphene are strongly interacting!

In general, lower dimensions enhance correlations.

SYMMETRIES RELEVANT FOR LOW-D MATERIALS

- Time-reversal symmetry T : $T^2 = \pm 1$

$$t \rightarrow -t \implies E(k) = E(-k)$$

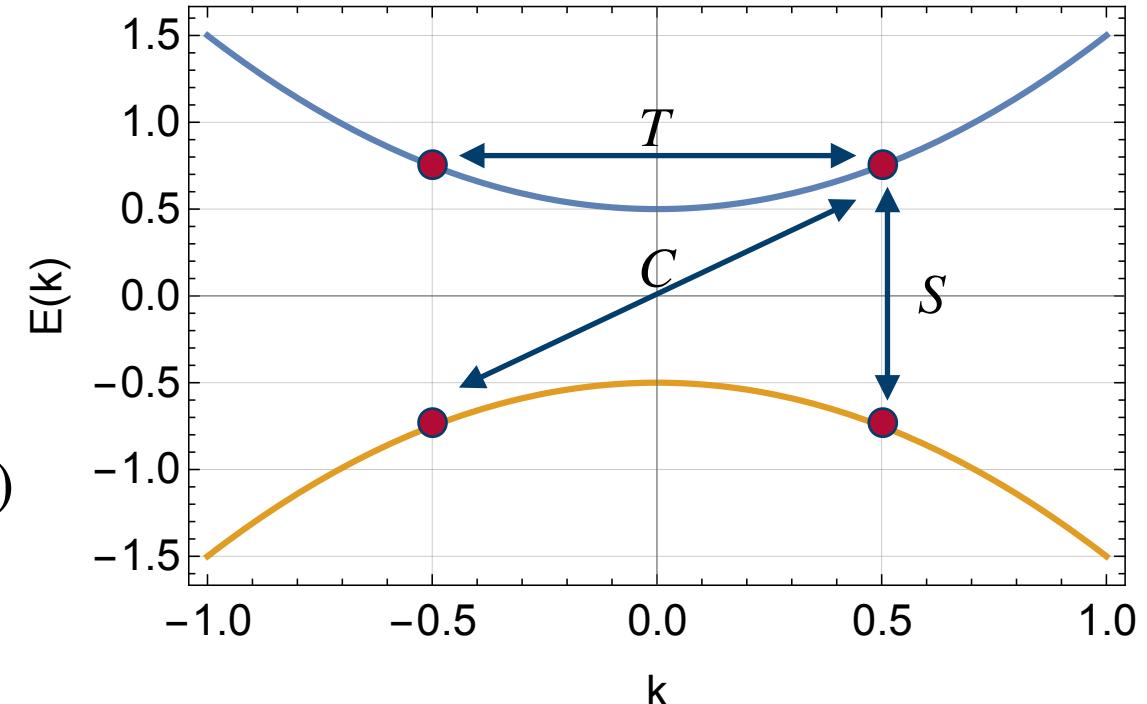
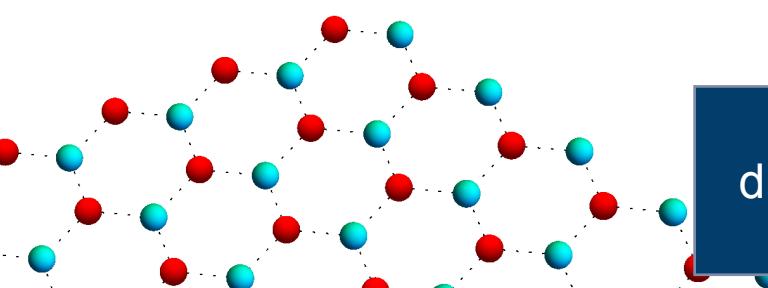
- Charge conjugation symmetry (or *particle-hole* symmetry) C : $C^2 = \pm 1$

Spectrum symmetric about zero: $E_+(k) = -E_-(-k)$

- Chiral symmetry (or *sublattice* symmetry)

$$S: S^2 = S$$

$$E_+(k) = -E_-(k)$$

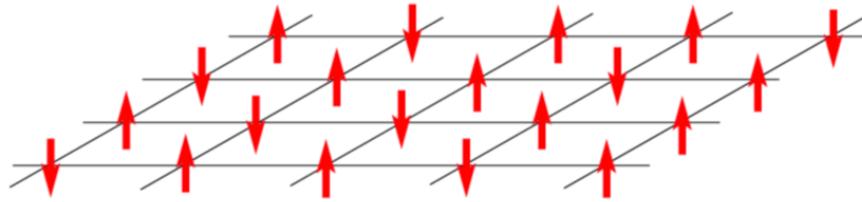


Normally, different phases of matter are distinguished by their ground-state symmetries (and lack thereof)

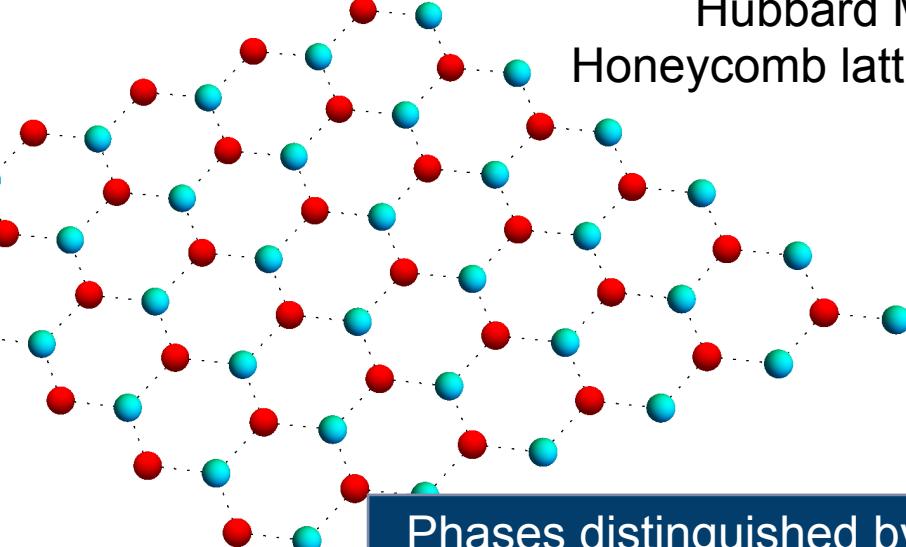
SYMMETRY BREAKING AND PHASES OF MATTER

... and the transitions between them ...

Ising Model

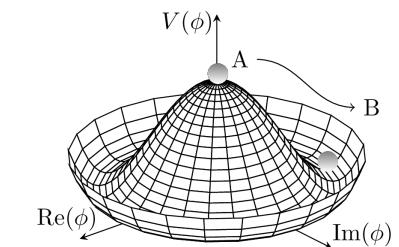
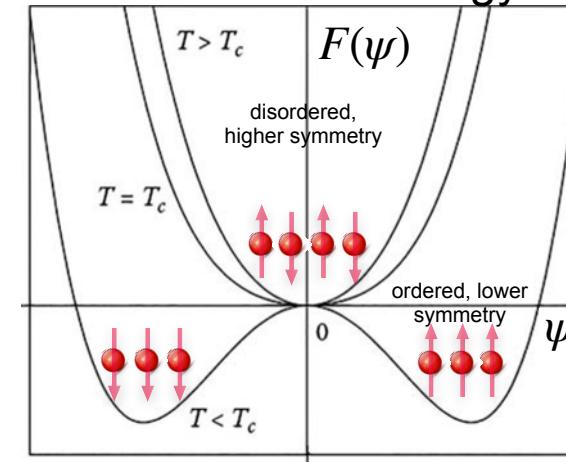


Hubbard Model on
Honeycomb lattice (graphene)



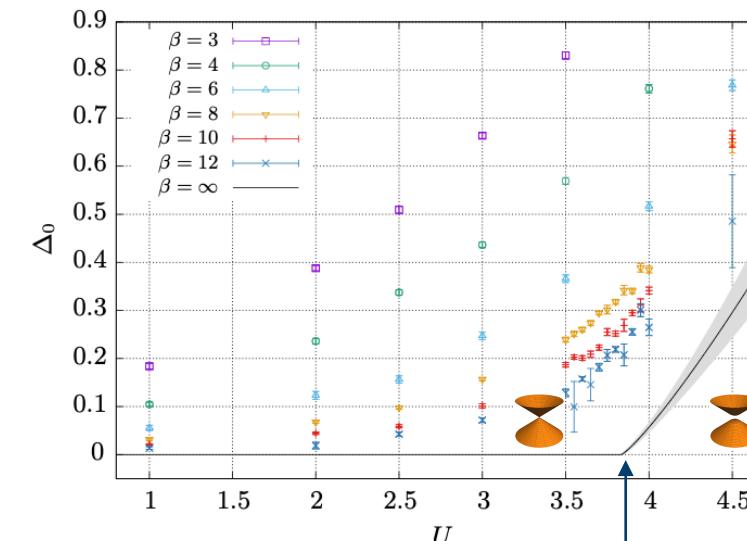
Phases distinguished by
different symmetries

Landau Free Energy



Continuous order parameter
in a discrete system?

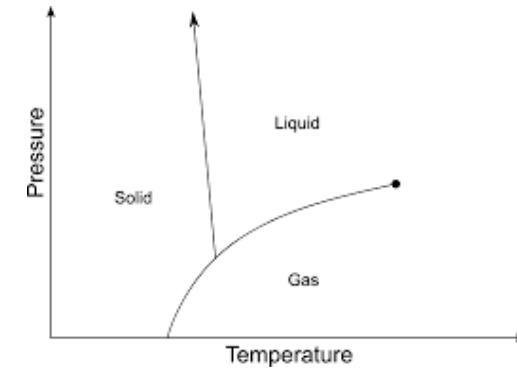
J. Ostmeyer, T.L., et al. [arXiv:1912.03278]
Comput.Phys.Commun. **265** (2021) 107978



Most accurate prediction of critical coupling: $U_c = 3.834(14)$

PHASES OF MATTER THAT SHARE THE SAME SYMMETRIES

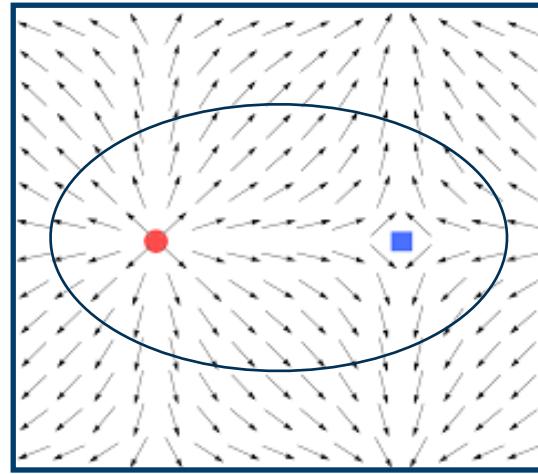
Classic example: liquid/gas transition



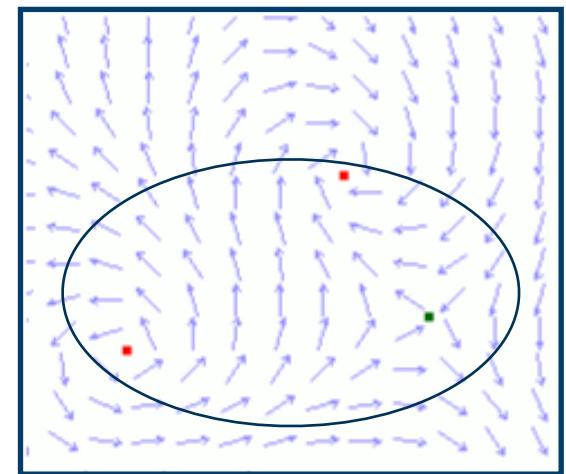
Another example: BKT transition (XY-Model)

Phases classified by local topological invariant

$$\pi_1(S^1) = \mathbb{Z} \text{ (ie winding number)}$$



$$J < J_c \\ |\nu| = 0 \in \mathbb{Z}$$



$$J > J_c \\ |\nu| = 1 \in \mathbb{Z}$$

Phases are distinct, but the ground states do not break the symmetry of the system

MERMIN-WAGNER THEOREM

continuous symmetries cannot be spontaneously broken at finite temperature in systems with sufficiently short-range interactions in dimensions $d \leq 2$

MERMIN-WAGNER THEOREM

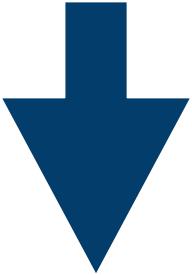
continuous symmetries cannot be spontaneously broken at finite temperature in systems with sufficiently short-range interactions in dimensions $d \leq 2$



no goldstone modes!

MERMIN-WAGNER THEOREM

continuous symmetries cannot be spontaneously broken at finite temperature in systems with sufficiently short-range interactions in dimensions $d \leq 2$



no goldstone modes!

Phases of matter classified topologically

THUS TOPOLOGY CAN ALSO DISTINGUISH PHASES OF MATTER

But what does “topology” mean in this case?

THUS TOPOLOGY CAN ALSO DISTINGUISH PHASES OF MATTER

But what does “topology” mean in this case?

Topological Geometry



THUS TOPOLOGY CAN ALSO DISTINGUISH PHASES OF MATTER

But what does “topology” mean in this case?

Topological Geometry



~



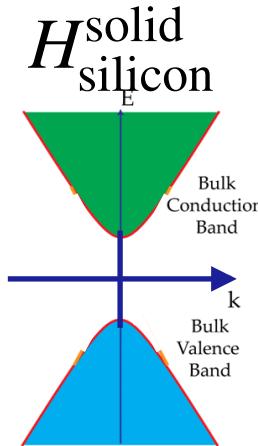
✗



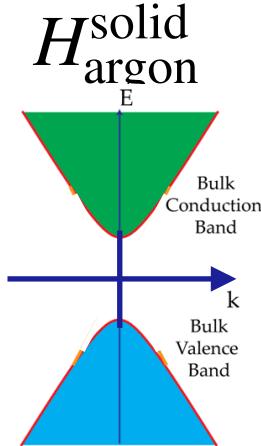
~



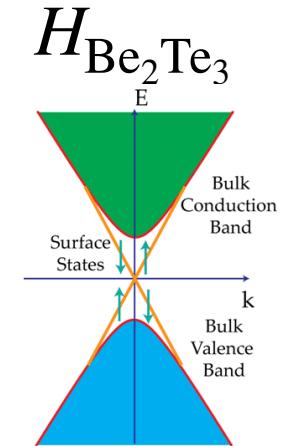
Topological Matter



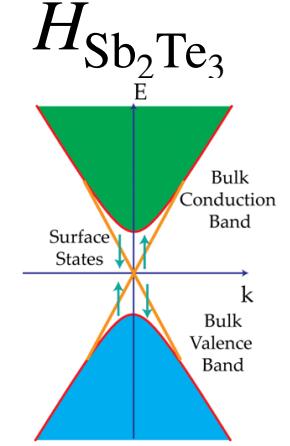
~



✗



~



THUS TOPOLOGY CAN ALSO DISTINGUISH PHASES OF MATTER

But what does “topology” mean in this case?

Topological Geometry



~



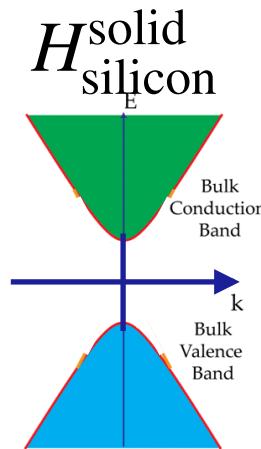
✗



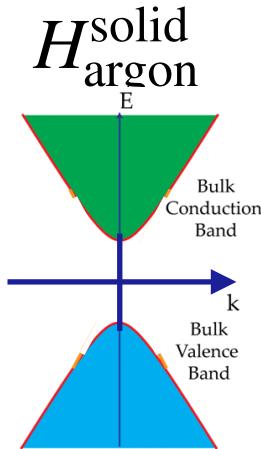
~



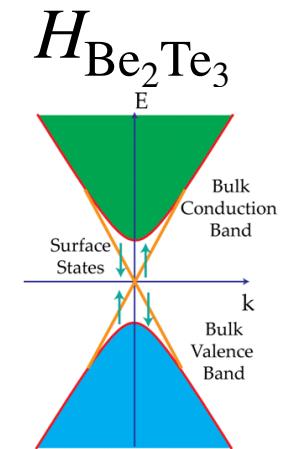
Topological Matter



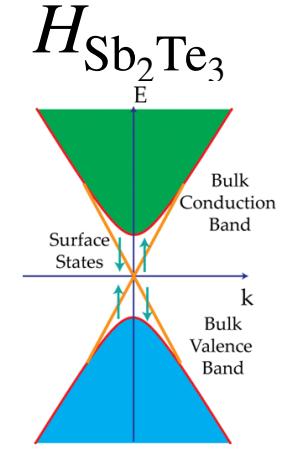
~



✗



~



CLASSIFICATION OF MATTER: *THE TEN-FOLD WAY*

. . . aka having ‘particle-physics envy’ . . .

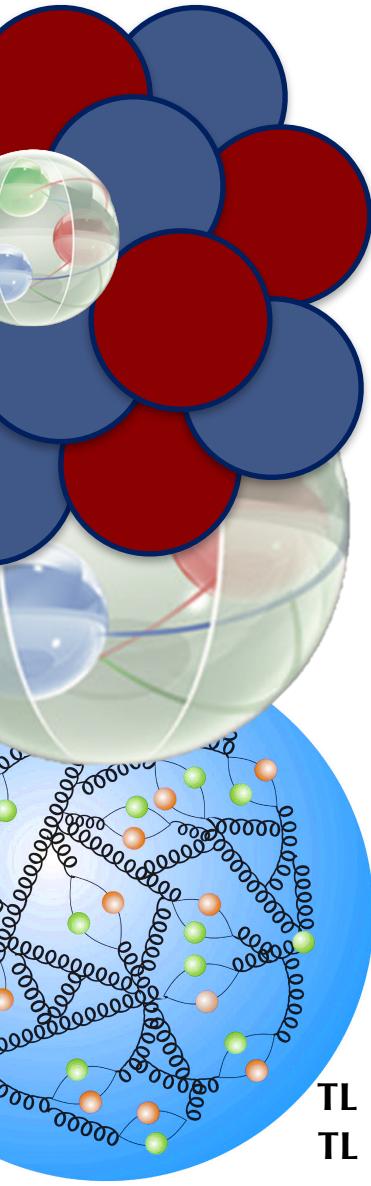
AZ	Symmetry			Dimension							
	T	C	S	1	2	3	4	5	6	7	8
A	0	0	0	0	\mathbb{Z}	0	\mathbb{Z}	0	\mathbb{Z}	0	\mathbb{Z}
AIII	0	0	1	\mathbb{Z}	0	\mathbb{Z}	0	\mathbb{Z}	0	\mathbb{Z}	0
AI	1	0	0	0	0	0	\mathbb{Z}	0	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}
BDI	1	1	1	\mathbb{Z}	0	0	0	\mathbb{Z}	0	\mathbb{Z}_2	\mathbb{Z}_2
D	0	1	0	\mathbb{Z}_2	\mathbb{Z}	0	0	0	\mathbb{Z}	0	\mathbb{Z}_2
DIII	-1	1	1	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}	0	0	0	\mathbb{Z}	0
AII	-1	0	0	0	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}	0	0	0	\mathbb{Z}
CII	-1	-1	1	\mathbb{Z}	0	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}	0	0	0
C	0	-1	0	0	\mathbb{Z}	0	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}	0	0
CI	1	-1	1	0	0	\mathbb{Z}	0	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}	0

Bott periodicity

NOVEL FORMS OF EMERGENT PHENOMENA



“Strong Emergentism” vs “Weak Emergentism”



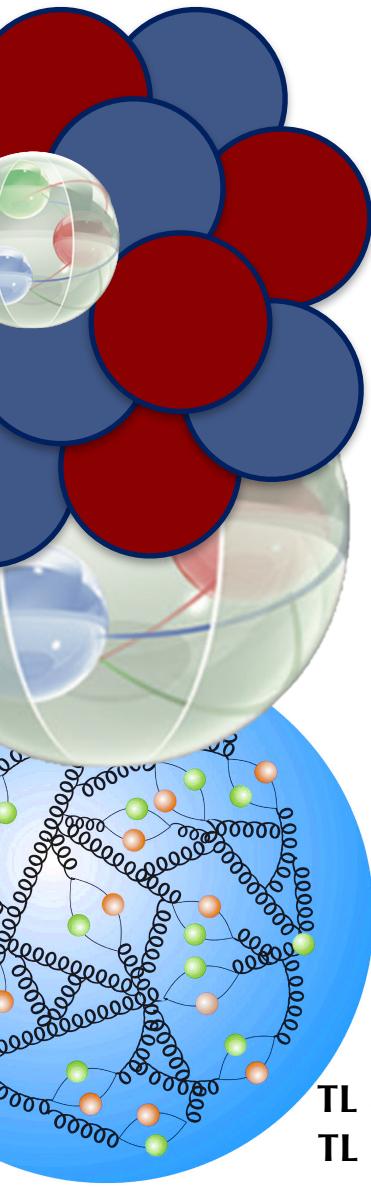
TL & U. Meißner, [arXiv:2007.10062] Found.Phys. **50** (2020) 1140

TL & U. Meißner, [arXiv:1910.13770] **Top-Down Causation & Emergence**, Springer Verlag (2021), pgs.101-114

NOVEL FORMS OF EMERGENT PHENOMENA



“Strong Emergentism” vs “Weak Emergentism”

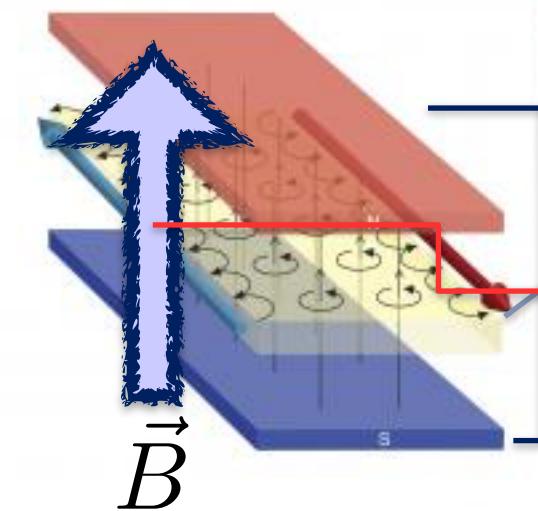


The (Fractional) Quantum Hall effect

Representation 1

QHE: Quantized cyclotron orbits

FQHE: Anyons (composite electrons)



Representation 2

Macro-state boundaries

Electrons in 2-dimensions

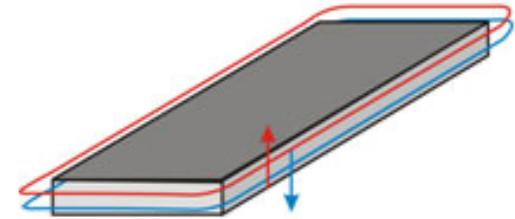
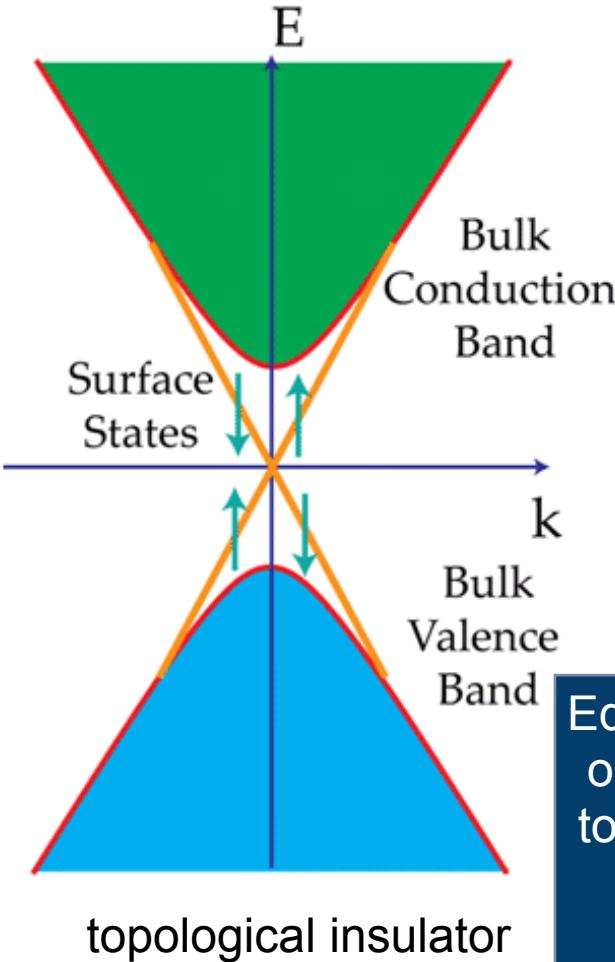
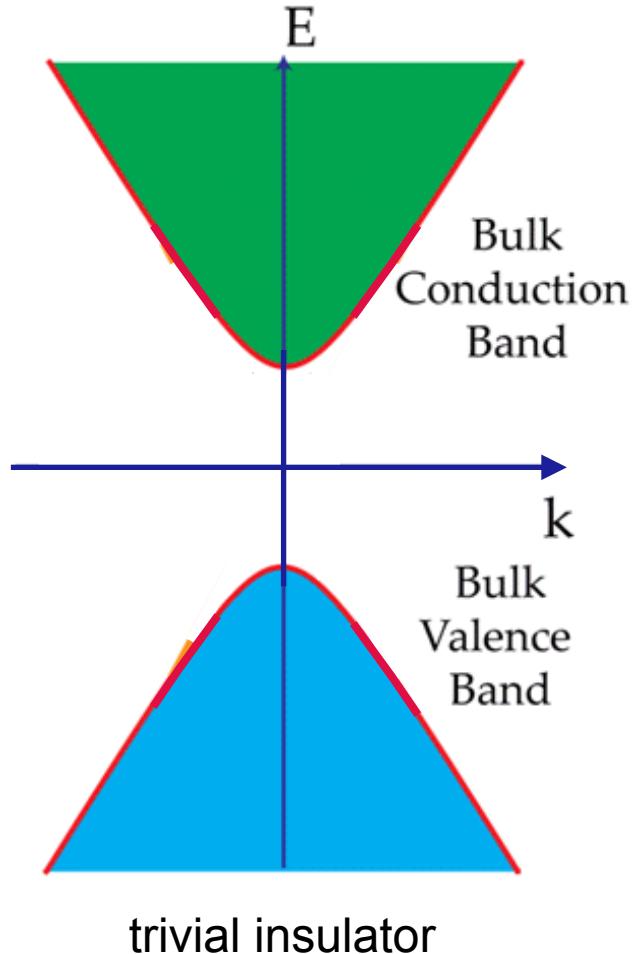
Macro-state magnetic field

All systems described by micro-level states, i.e. QED

Weak emergence is “... reducible in principle, but also *in principle irreducible in practice*”
(M. Bedau, 2010)

TOPOLOGICAL INSULATORS . . .

. . . and the bulk-boundary correspondence



2D topological insulator

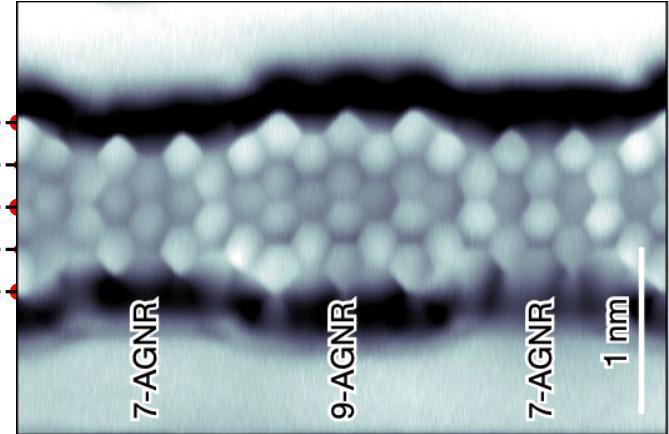
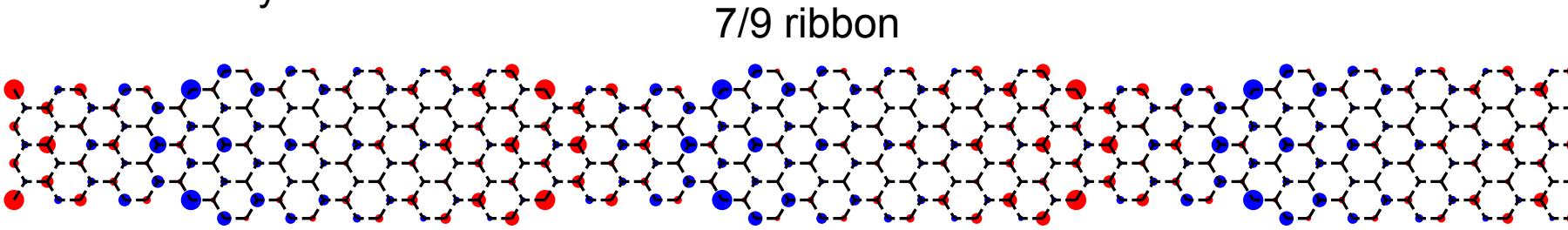
Edge/surface (localized) states occur at boundaries between topologically distinct materials

Localized states are “symmetry-protected”

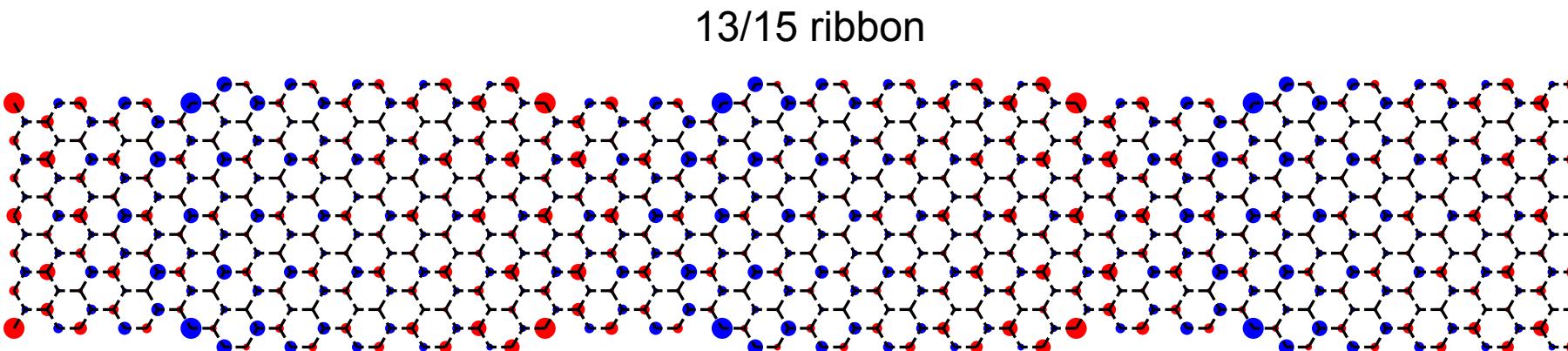
ANOTHER EXAMPLE OF LOCALIZATION

Hybrid nanoribbons

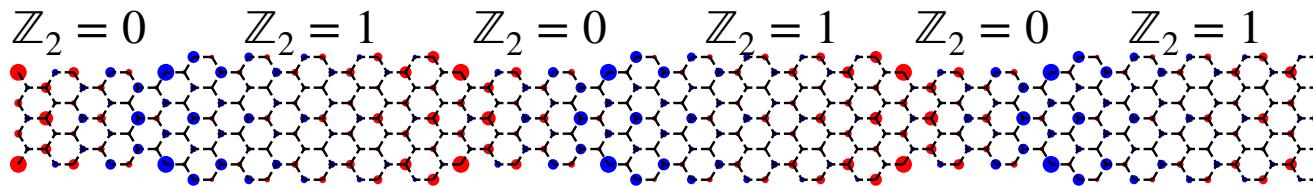
What is an hybrid nanoribbon?



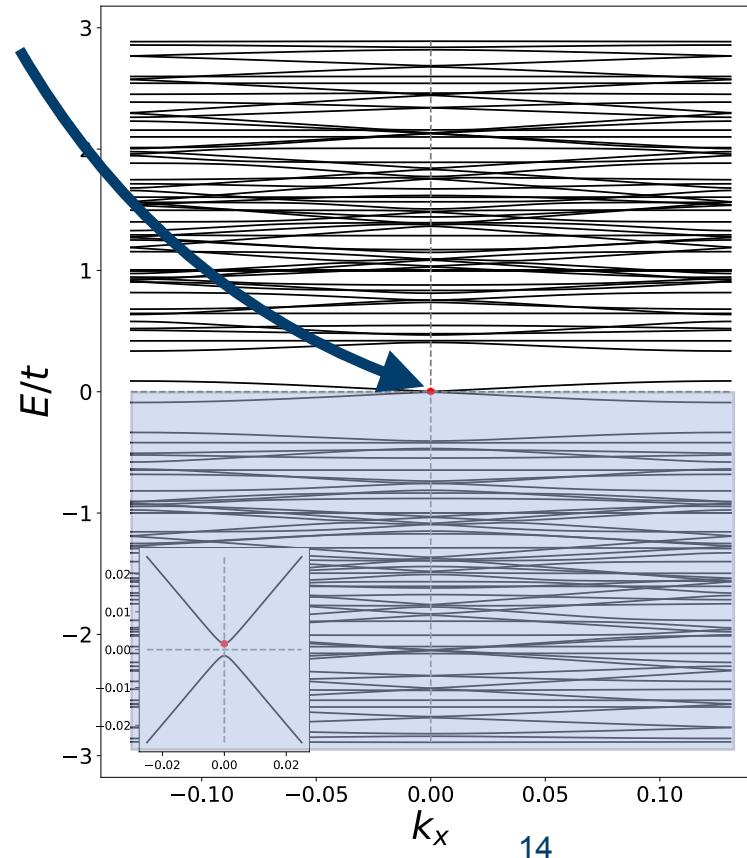
Rizzo, D.J., Veber, G., Cao, T. et al. Topological band engineering of graphene nanoribbons. *Nature* **560**, 204–208 (2018)



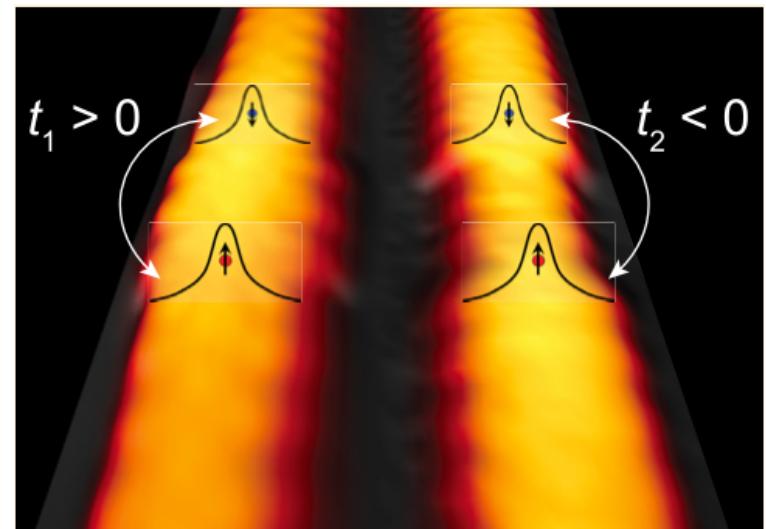
LOWEST ENERGY STATE EXHIBITS “LOCALIZATION”



Cao *et al.*, Phys. Rev. Lett. **119**, 076401 (2017)



Experimental evidence

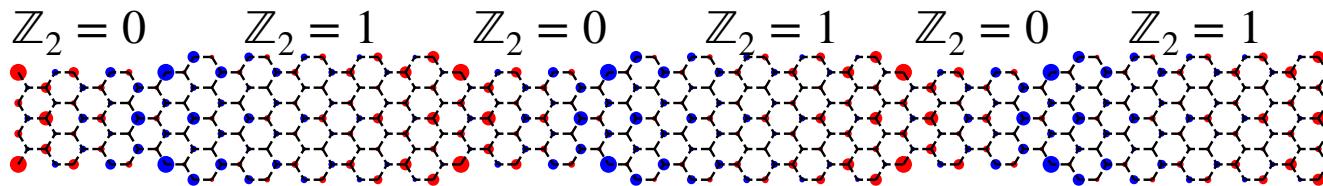


Rizzo *et al.*, ACS Nano 2021, 15, 12, 20633–20642

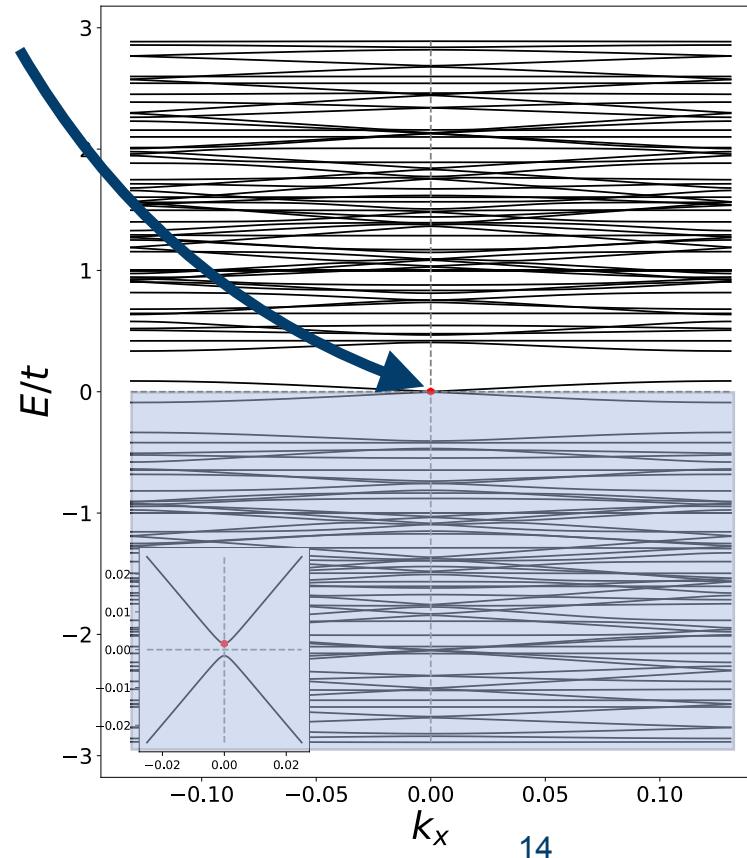
Potential application: Topological Quantum Dots

. . . and fault-tolerant quantum computing (one day)

LOWEST ENERGY STATE EXHIBITS “LOCALIZATION”

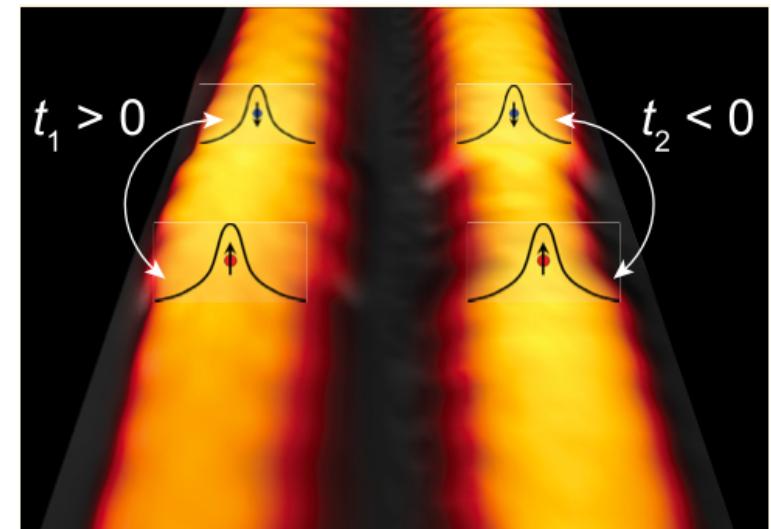


Cao *et al.*, Phys. Rev. Lett. **119**, 076401 (2017)



All theoretical analysis is based off *non-interacting* dynamics!

Experimental evidence



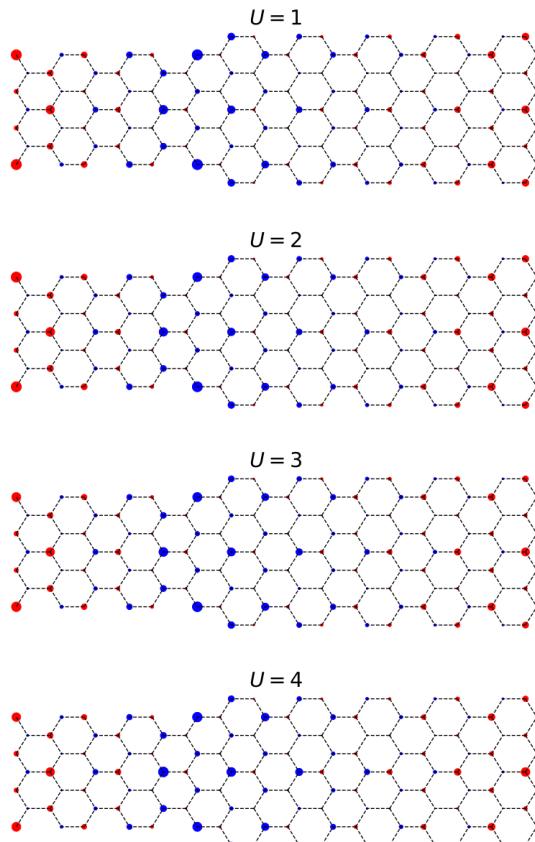
Rizzo *et al.*, ACS Nano 2021, 15, 12, 20633–20642

Potential application: Topological Quantum Dots

. . . and fault-tolerant quantum computing (one day)

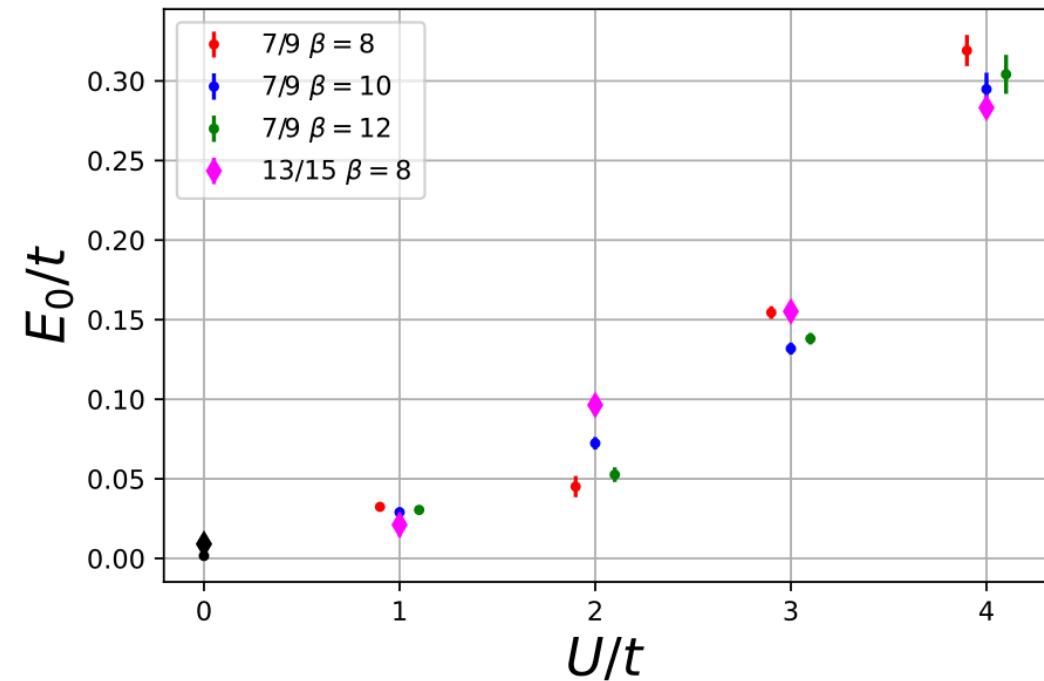
HOW DOES INTERACTION CHANGE THINGS?

Simulations with Quantum Monte Carlo



Localizations persist with strong interactions

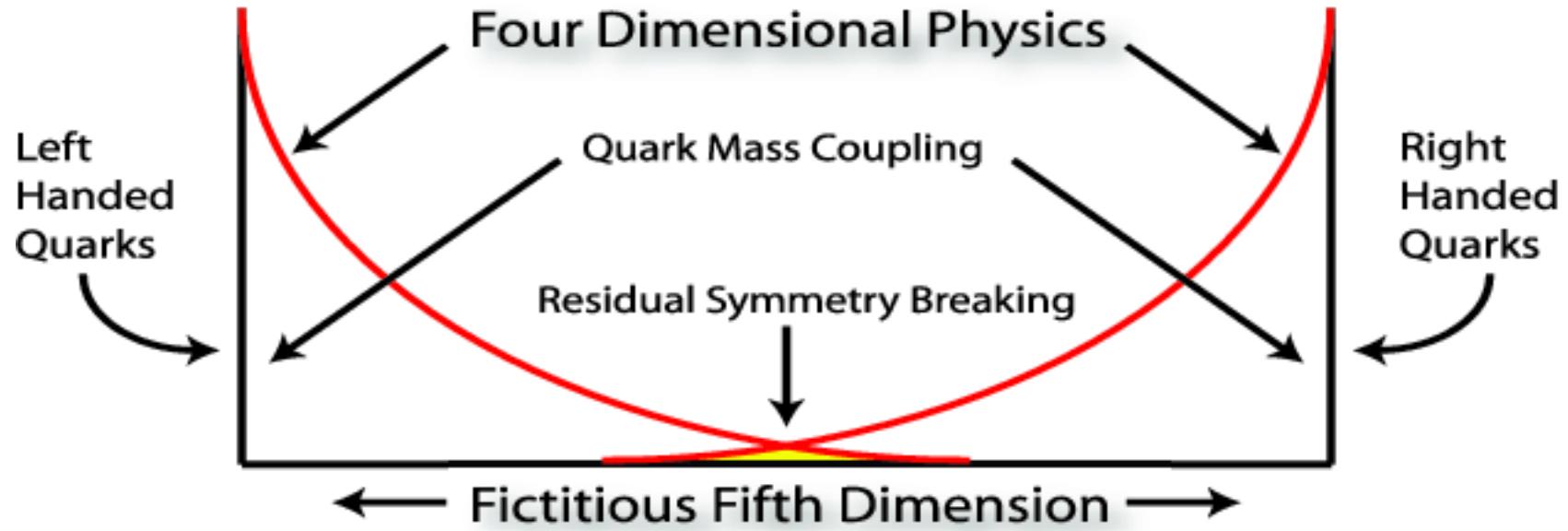
$$H = -t \sum_{\langle i,j \rangle, \sigma=\uparrow,\downarrow} (a_{i,\sigma}^\dagger a_{j\sigma} + \text{H.c}) + U \sum_i \left(n_{i,\uparrow} - \frac{1}{2} \right) \left(n_{i,\downarrow} - \frac{1}{2} \right)$$



But energy depends on U !

DO SUCH LOCALISATIONS LOOK FAMILIAR?

Domain-Wall fermions in LQCD

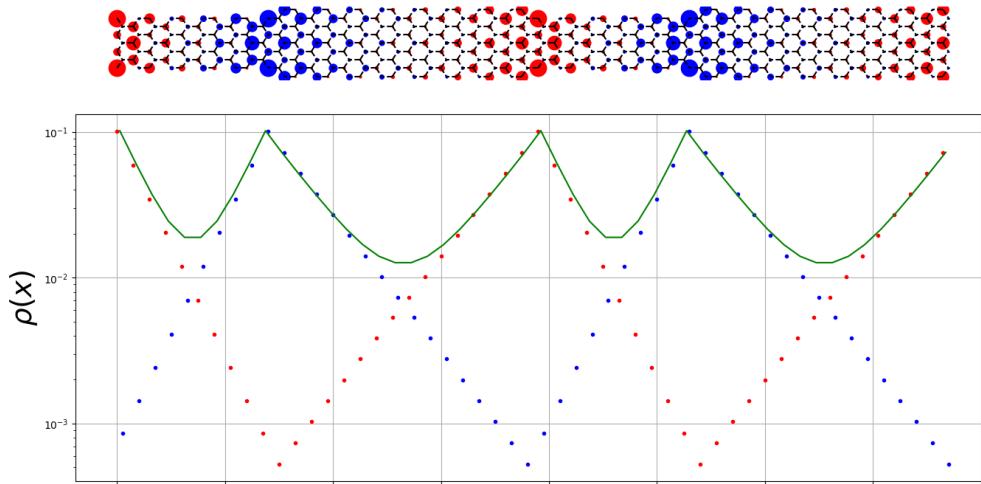


Hybrid ribbons provide physical manifestation of domain wall fermions

OUR INVESTIGATIONS LEAD US TO A NEW TYPE OF LOCALIZATION

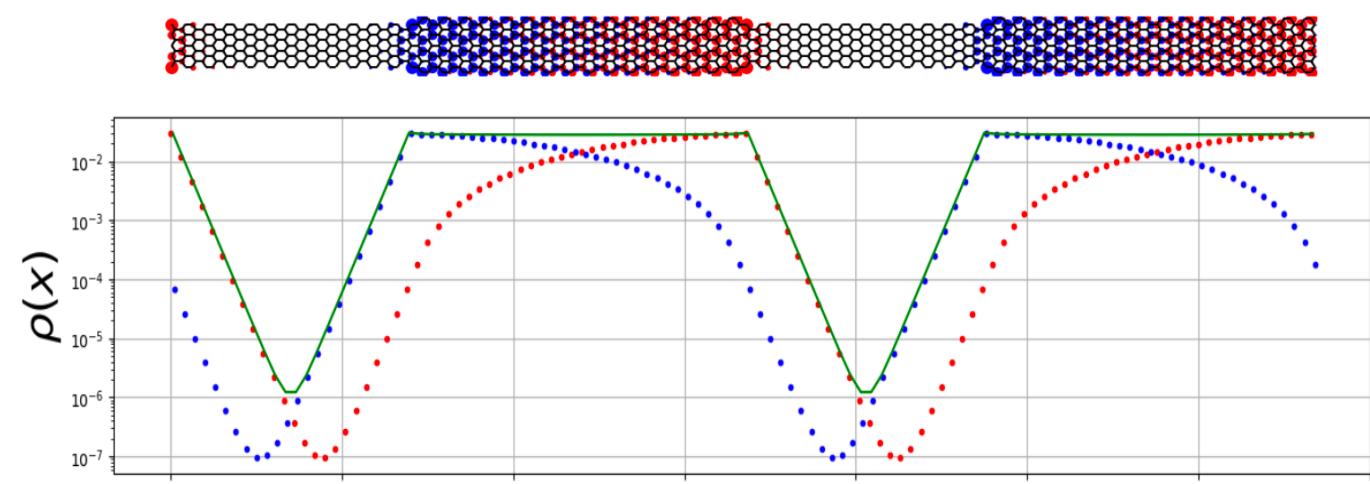
Fuji vs Kilimanjaro J. Ostmeyer, L. Razmadze, E. Berkowitz, **TL** & U.-G. Meißner, [arXiv:2401.04715] Phys.Rev.B 109 (2024) 195135

7/9 hybrid



Predicted from Cao *et al.*, Phys.
Rev. Lett. **119**, 076401 (2017)

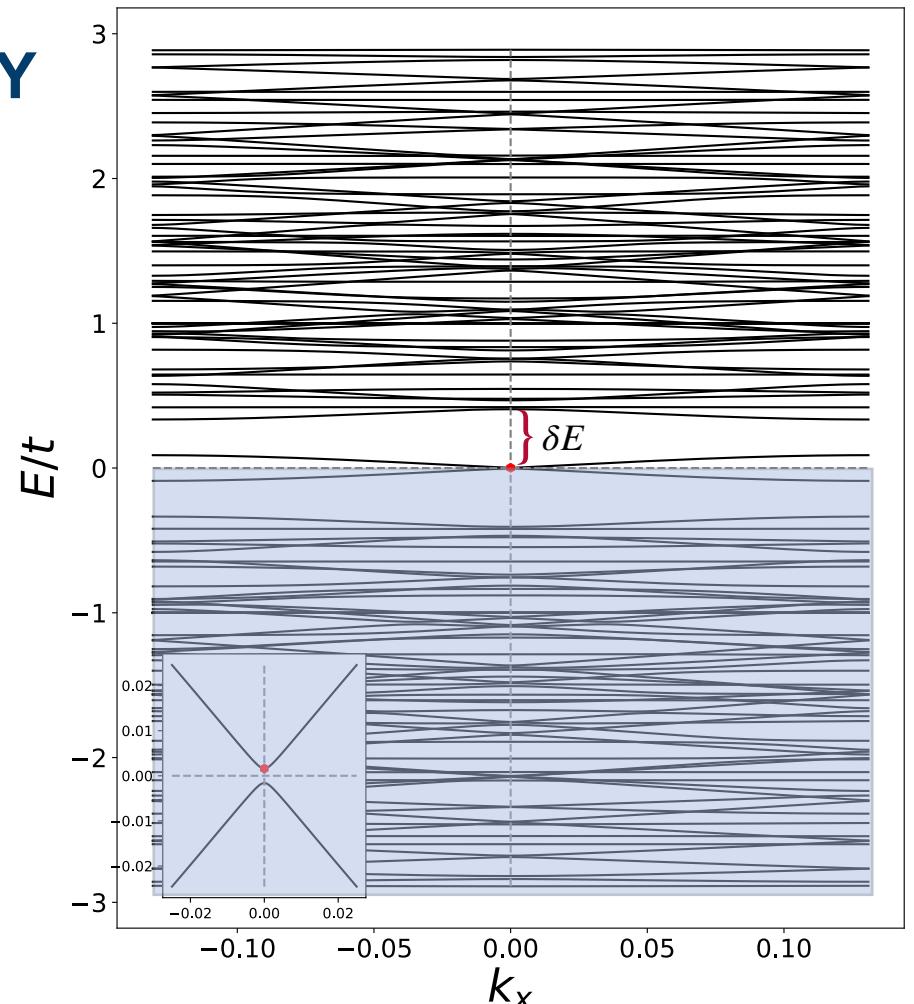
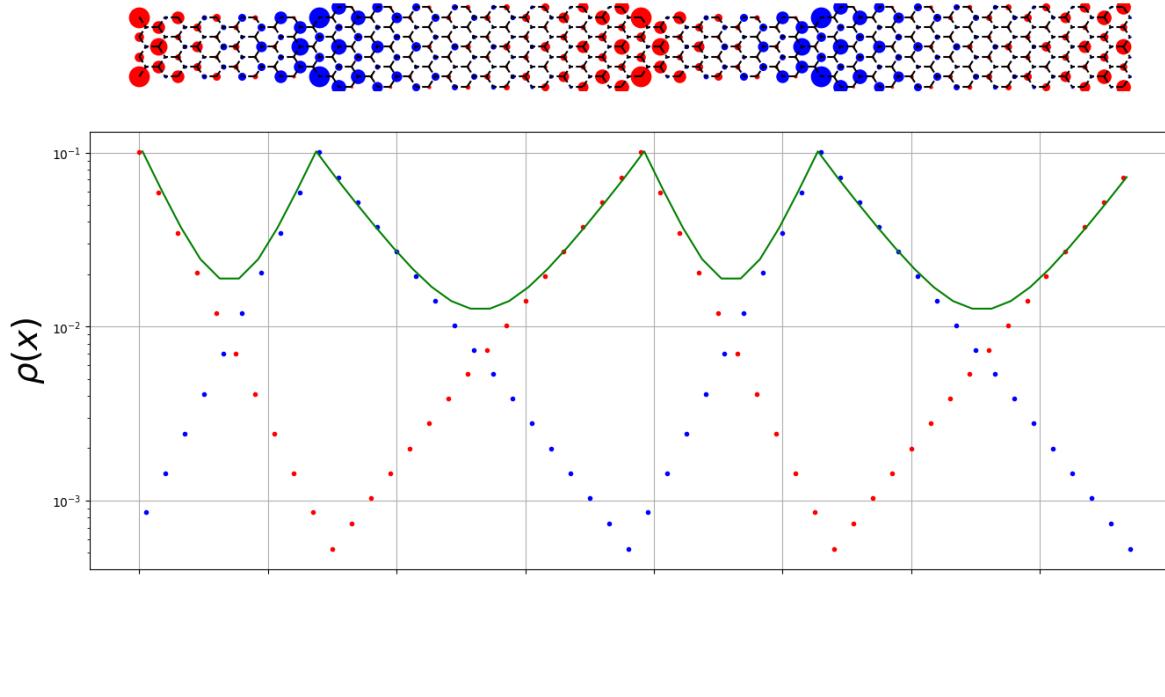
9/11 hybrid



Our addition to Cao *et al.*, Phys. Rev.
Lett. **119**, 076401 (2017)

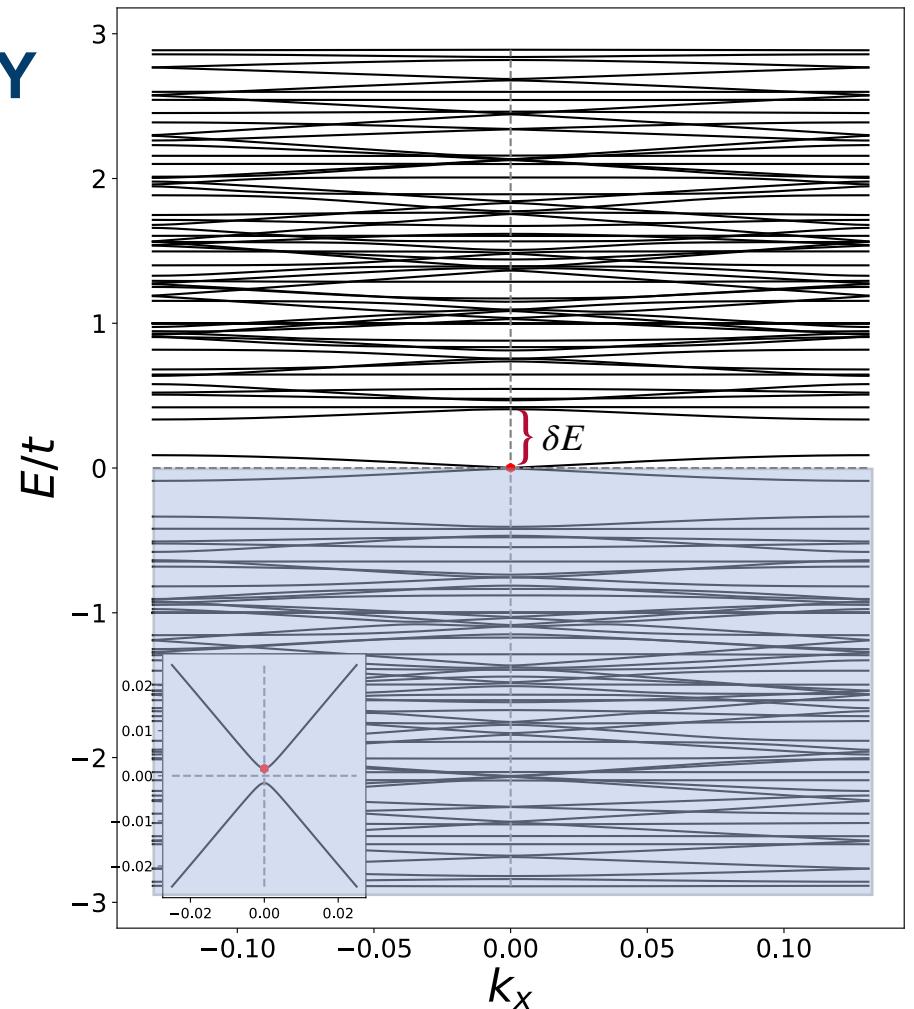
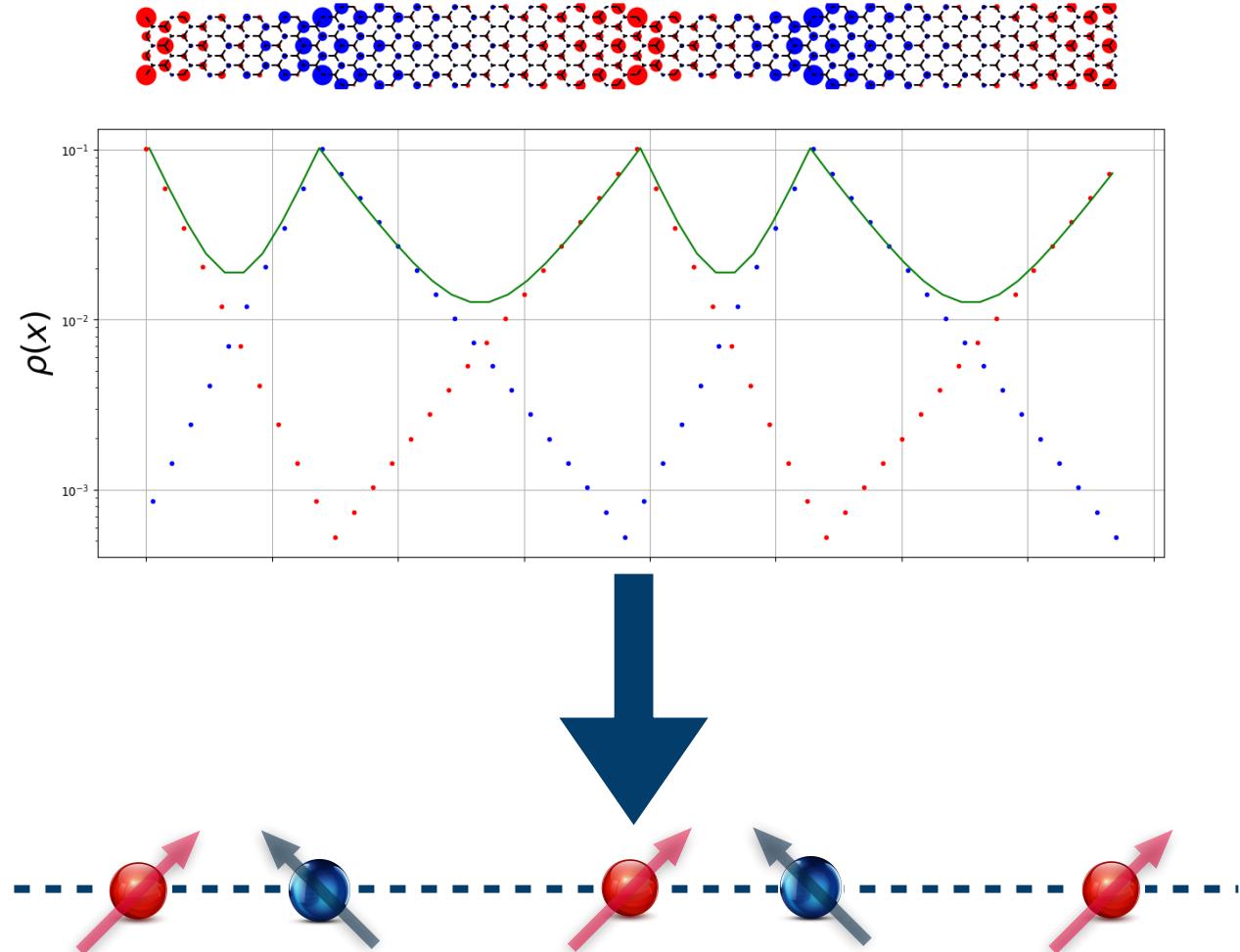
SUCH LOCALIZATIONS ALLOW US TO SIMPLIFY OUR THEORY

1-D effective theory



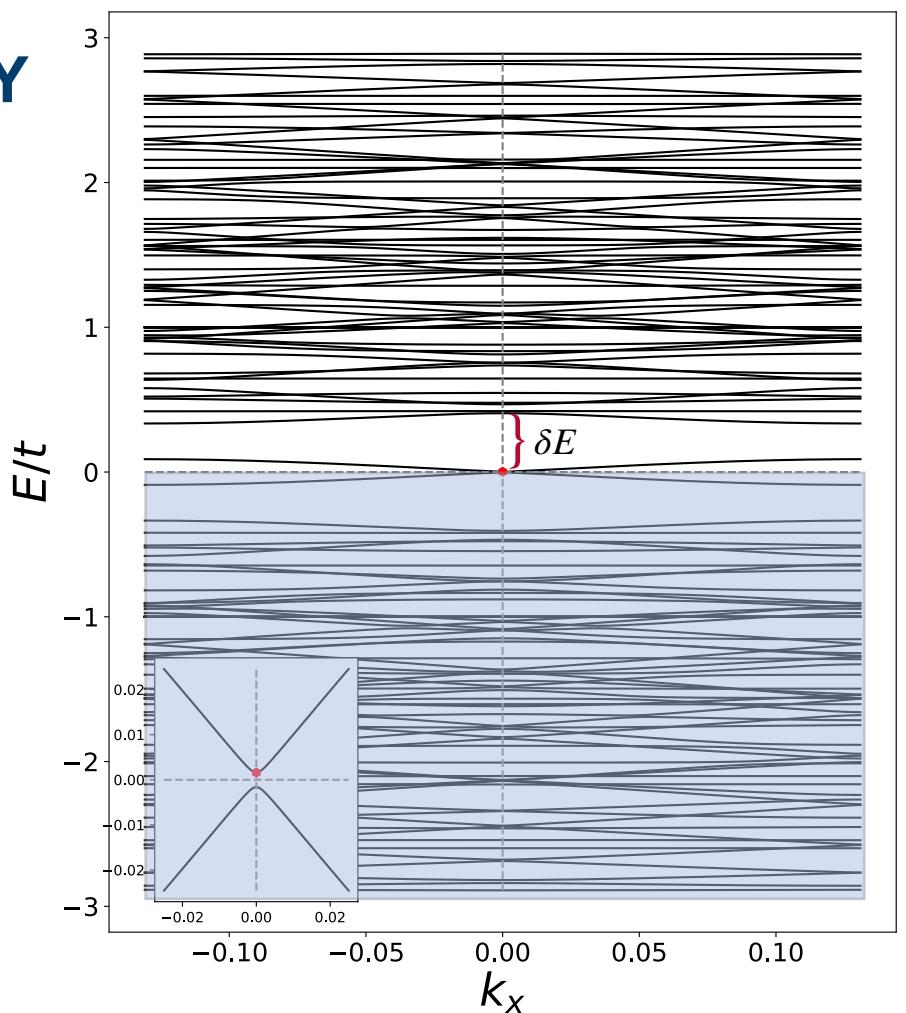
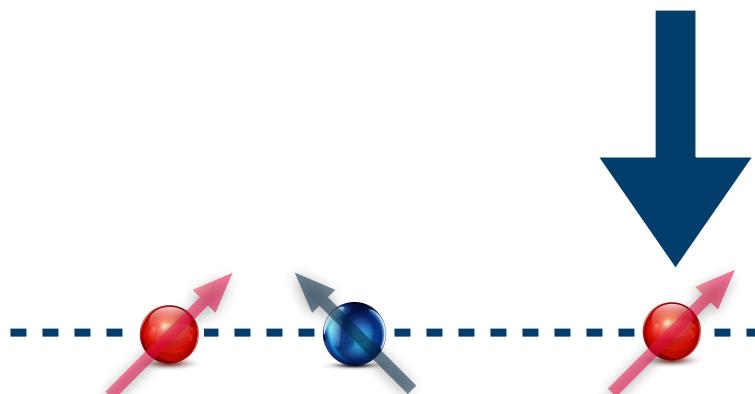
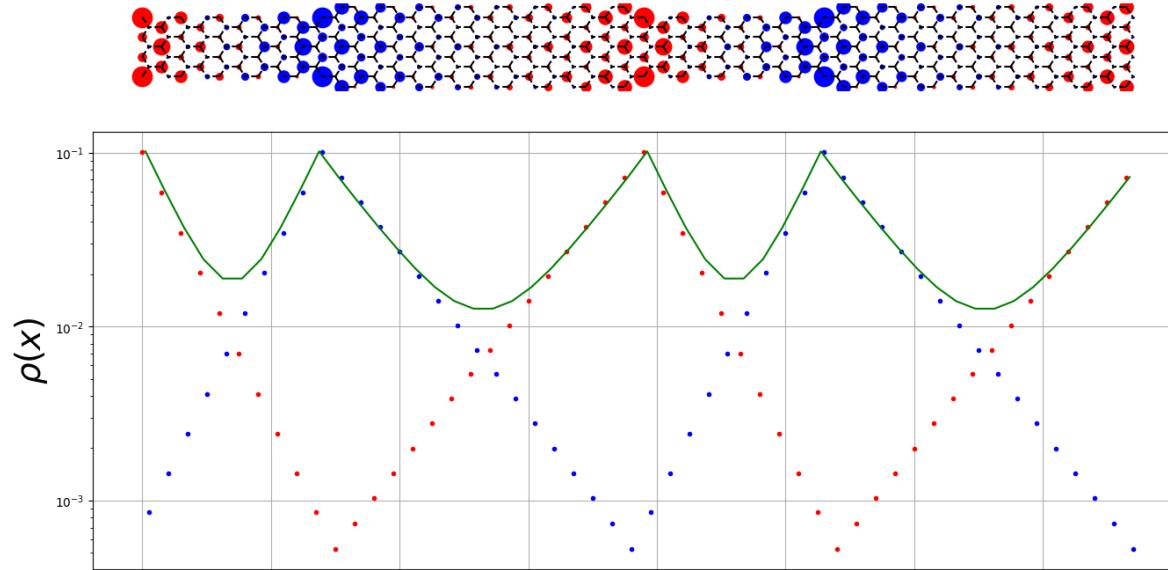
SUCH LOCALIZATIONS ALLOW US TO SIMPLIFY OUR THEORY

1-D effective theory



SUCH LOCALIZATIONS ALLOW US TO SIMPLIFY OUR THEORY

1-D effective theory



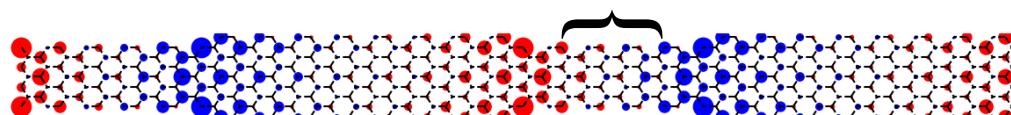
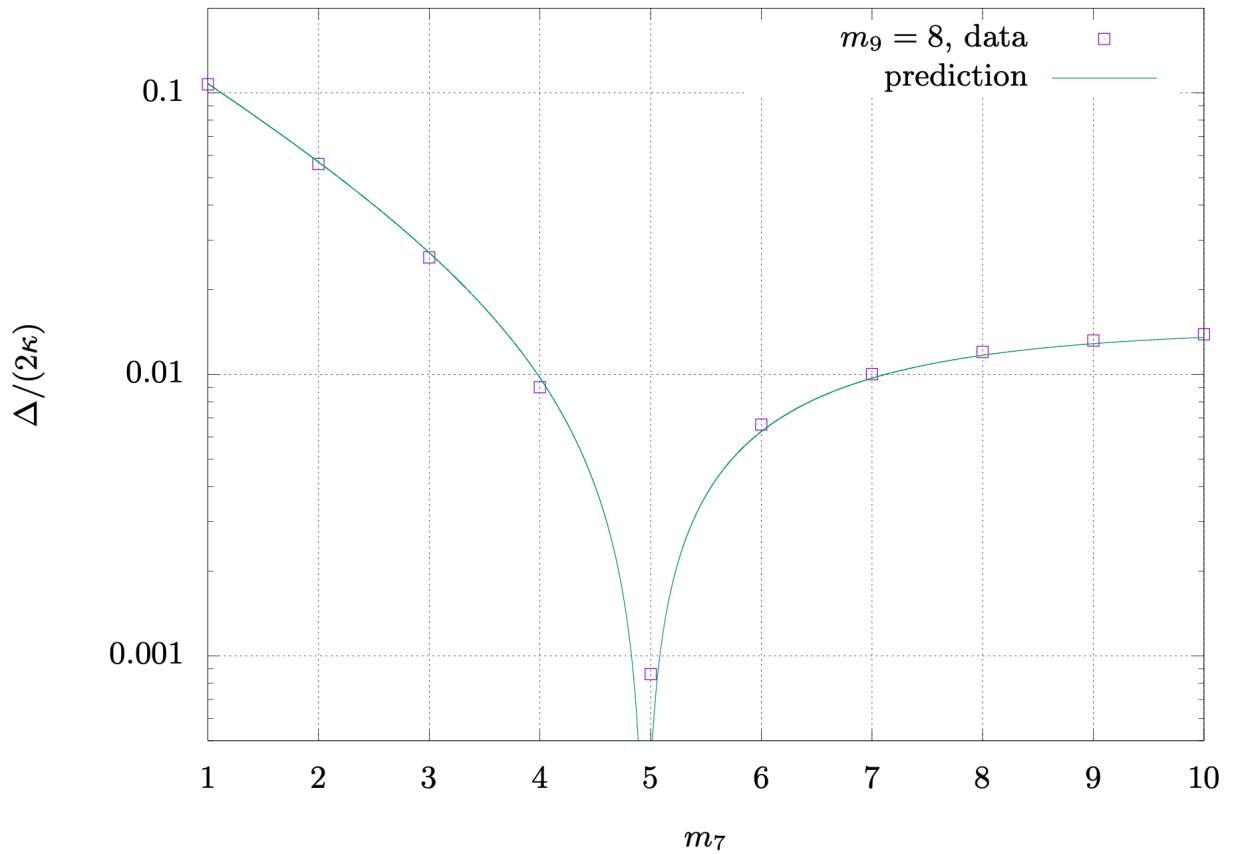
Low-energy ET

$$H_{1D} = - \sum_i \left(t_A a_{2i}^\dagger a_{2i-1} + t_B a_{2i+1}^\dagger a_{2i+2} + \text{H.c.} \right)$$

TUNING LOW-ENERGY CONSTANTS (LECS)

$$H_{1D} = - \sum_i \left(t_A a_{2i}^\dagger a_{2i-1} + t_B a_{2i+1}^\dagger a_{2i+2} + \text{H.c.} \right) = - \sum_k a_k^\dagger \begin{pmatrix} 0 & t_A e^{ik} + t_B e^{-ik} \\ t_A e^{-ik} + t_B e^{ik} & 0 \end{pmatrix} a_k$$

- Match t_A and t_B to underlying theory with a particular geometry
- Predict low-energy spectrum of different geometries



INCLUDING INTERACTIONS WITHIN OUR ET

- Localization persists in the presence of interactions
- Energy gap is symmetric about Fermi energy
 - particle/hole & chiral symmetries
 - \implies Inclusion of staggered mass $m_s \sigma_3$ (LEC) into ET

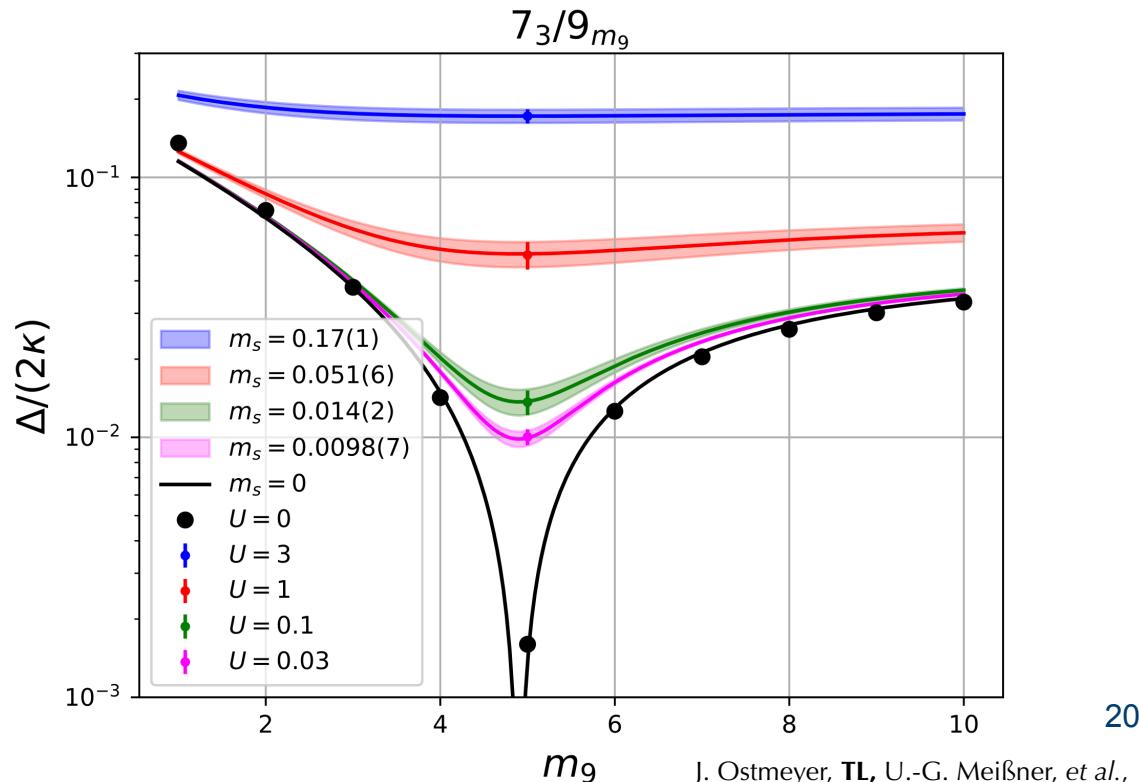
$$H_{1D} = - \sum_k a_k^\dagger \begin{pmatrix} m_s & t_A e^{ik} + t_B e^{-ik} \\ t_A e^{-ik} + t_B e^{ik} & -m_s \end{pmatrix} a_k$$

INCLUDING INTERACTIONS WITHIN OUR ET

- Localization persists in the presence of interactions
- Energy gap is symmetric about Fermi energy
 - particle/hole & chiral symmetries
 - \implies Inclusion of staggered mass $m_s \sigma_3$ (LEC) into ET

$$H_{1D} = - \sum_k a_k^\dagger \begin{pmatrix} m_s & t_A e^{ik} + t_B e^{-ik} \\ t_A e^{-ik} + t_B e^{ik} & -m_s \end{pmatrix} a_k$$

Tune m_s to underlying theory

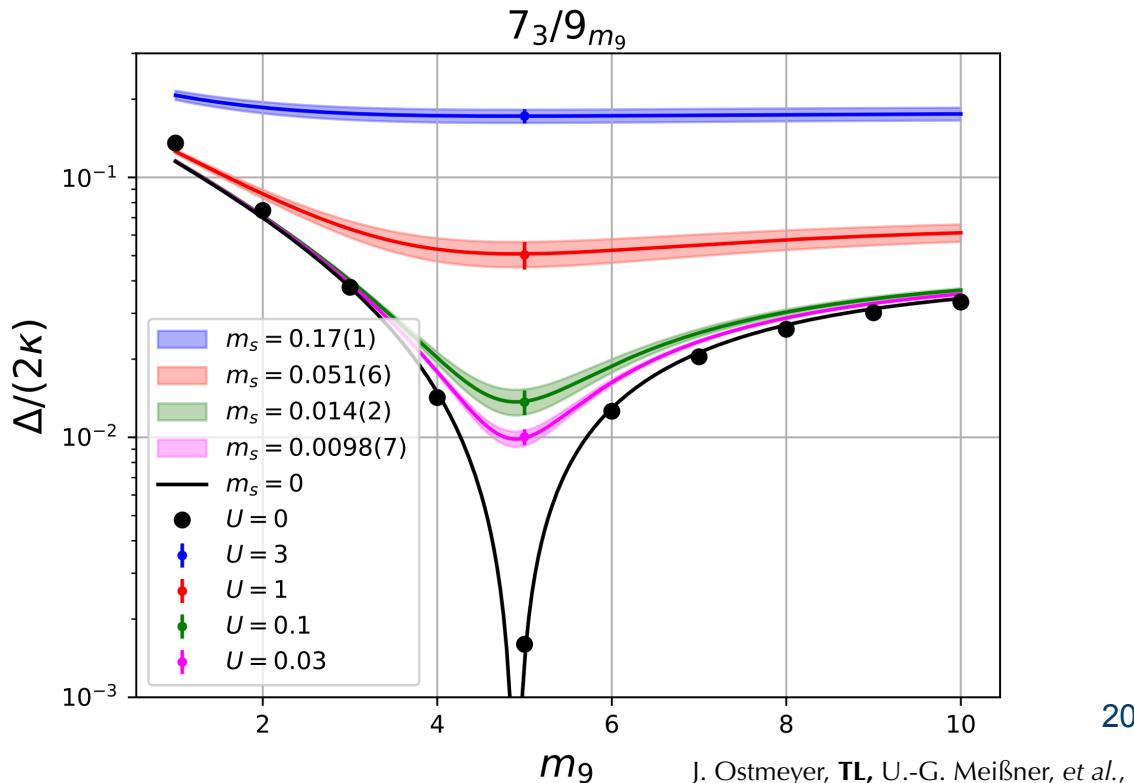


INCLUDING INTERACTIONS WITHIN OUR ET

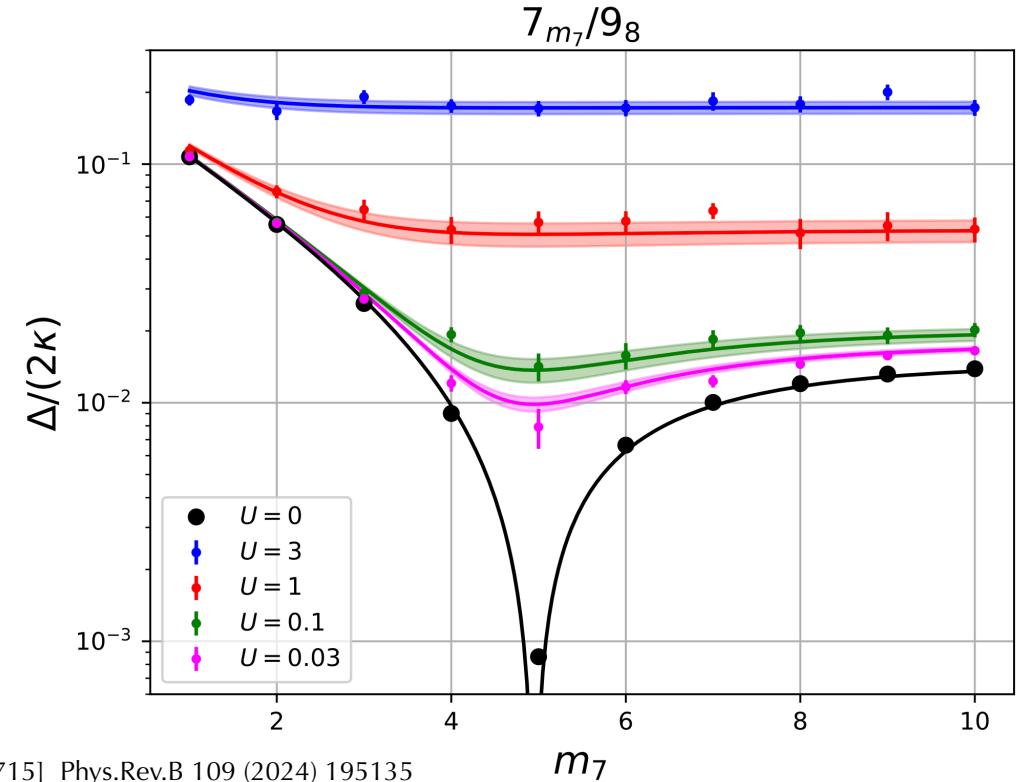
- Localization persists in the presence of interactions
- Energy gap is symmetric about Fermi energy
 - particle/hole & chiral symmetries
 - \implies Inclusion of staggered mass $m_s \sigma_3$ (LEC) into ET

$$H_{1D} = - \sum_k a_k^\dagger \begin{pmatrix} m_s & t_A e^{ik} + t_B e^{-ik} \\ t_A e^{-ik} + t_B e^{ik} & -m_s \end{pmatrix} a_k$$

Tune m_s to underlying theory

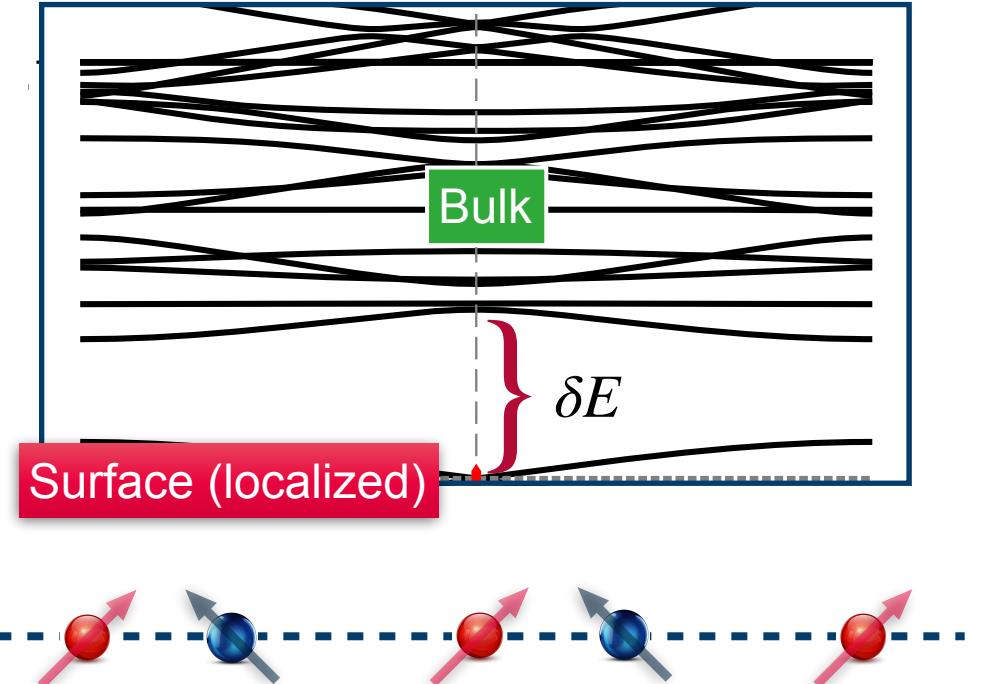


Predict spectrum of new geometries



INGREDIENTS FOR AN EFT

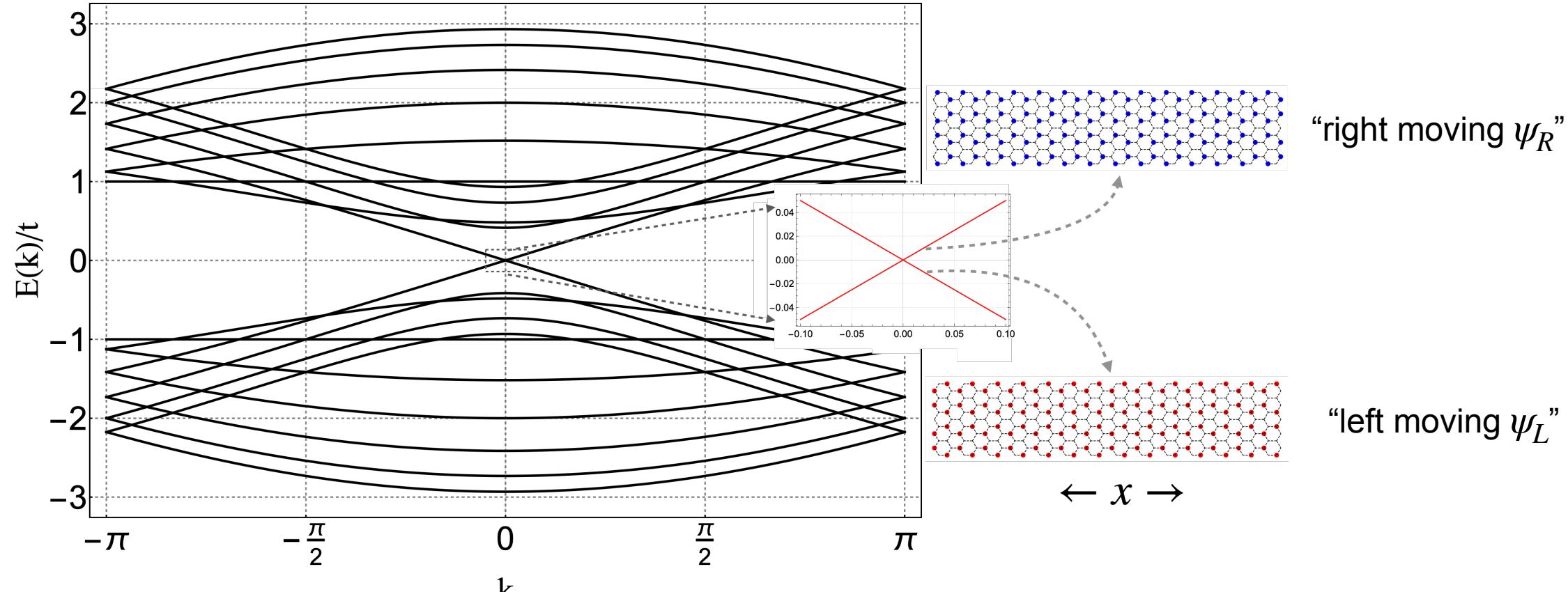
- Separation of scales (ie energy gap to bulk states)
- Identification of relevant low-energy degrees of freedom
- Interactions terms constrained by symmetries



$$\delta H_{T,C,S}^i + \mathcal{O}\left(\left(\frac{q}{\delta E}\right)^{i+1}\right)$$

ANOTHER EXAMPLE

Pure armchair nano ribbon (w/ width = 11)



Low-energy (non-interacting) dispersion $E(k) = \pm v_f k$

LOW-ENERGY EFT

... of a quantum wire ...

- Low-energy degrees of freedom in two-component form
- Lagrangian that captures correct low-energy dispersion
- States are electrically charged! Can include U(1) vector fields A_μ to describe interactions

$$\psi = \begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix}$$

$$\mathcal{L}_{\text{EFT}} = \bar{\psi} \left(i\gamma_0 \partial_t + iv_f \gamma_1 \partial_x \right) \psi$$
$$\gamma_0 = \sigma_2 \quad \gamma_1 = i\sigma_1 \quad \bar{\psi} = \psi^\dagger \gamma_0$$

$$\mathcal{L}_{\text{EFT}} + \mathcal{L}_{\text{QED}} = \bar{\psi} \left(i\gamma_0 (\partial_t - ieA_0(x)) + iv_f \gamma_1 (\partial_x - ieA_1(x)) \right) \psi - \frac{1}{4} F_{\mu\nu} F^{\mu\nu}$$

LOW-ENERGY EFT

... of a quantum wire ...

- Low-energy degrees of freedom in two-component form

$$\psi = \begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix}$$

- Lagrangian that captures correct low-energy dispersion

$$\mathcal{L}_{\text{EFT}} = \bar{\psi} \left(i\gamma_0 \partial_t + iv_f \gamma_1 \partial_x \right) \psi$$
$$\gamma_0 = \sigma_2 \quad \gamma_1 = i\sigma_1 \quad \bar{\psi} = \psi^\dagger \gamma_0$$

- States are electrically charged! Can include U(1) vector fields A_μ to describe interactions

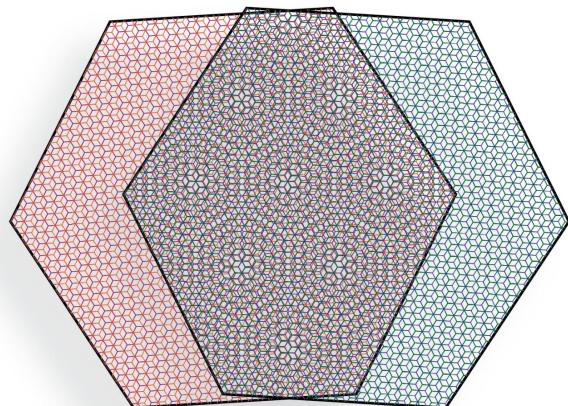
$$\mathcal{L}_{\text{EFT}} + \mathcal{L}_{\text{QED}} = \bar{\psi} \left(i\gamma_0 (\partial_t - ieA_0(x)) + iv_f \gamma_1 (\partial_x - ieA_1(x)) \right) \psi - \frac{1}{4} F_{\mu\nu} F^{\mu\nu}$$

QED in 1+1 dimensions: massless Schwinger model with fermi velocity v_f

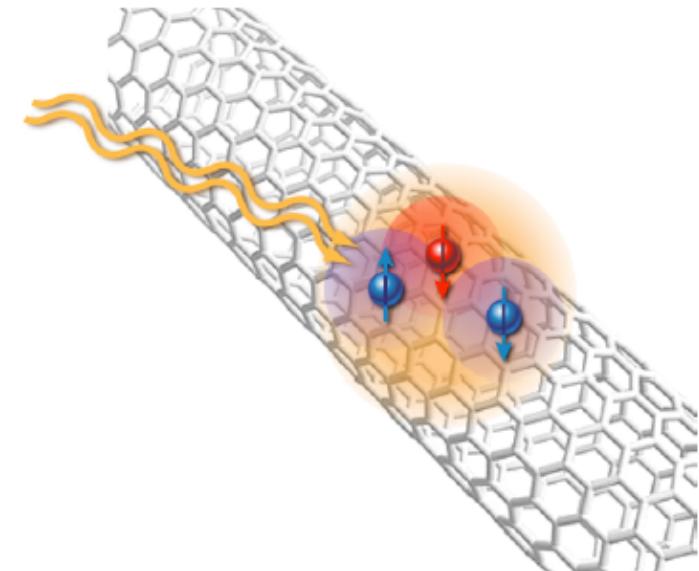
$$\implies m_s = \frac{ev_f}{\sqrt{\pi}}$$

OTHER EXAMPLES OF EMERGENT PHENOMENA

Superconductivity in bilayers
with a twist



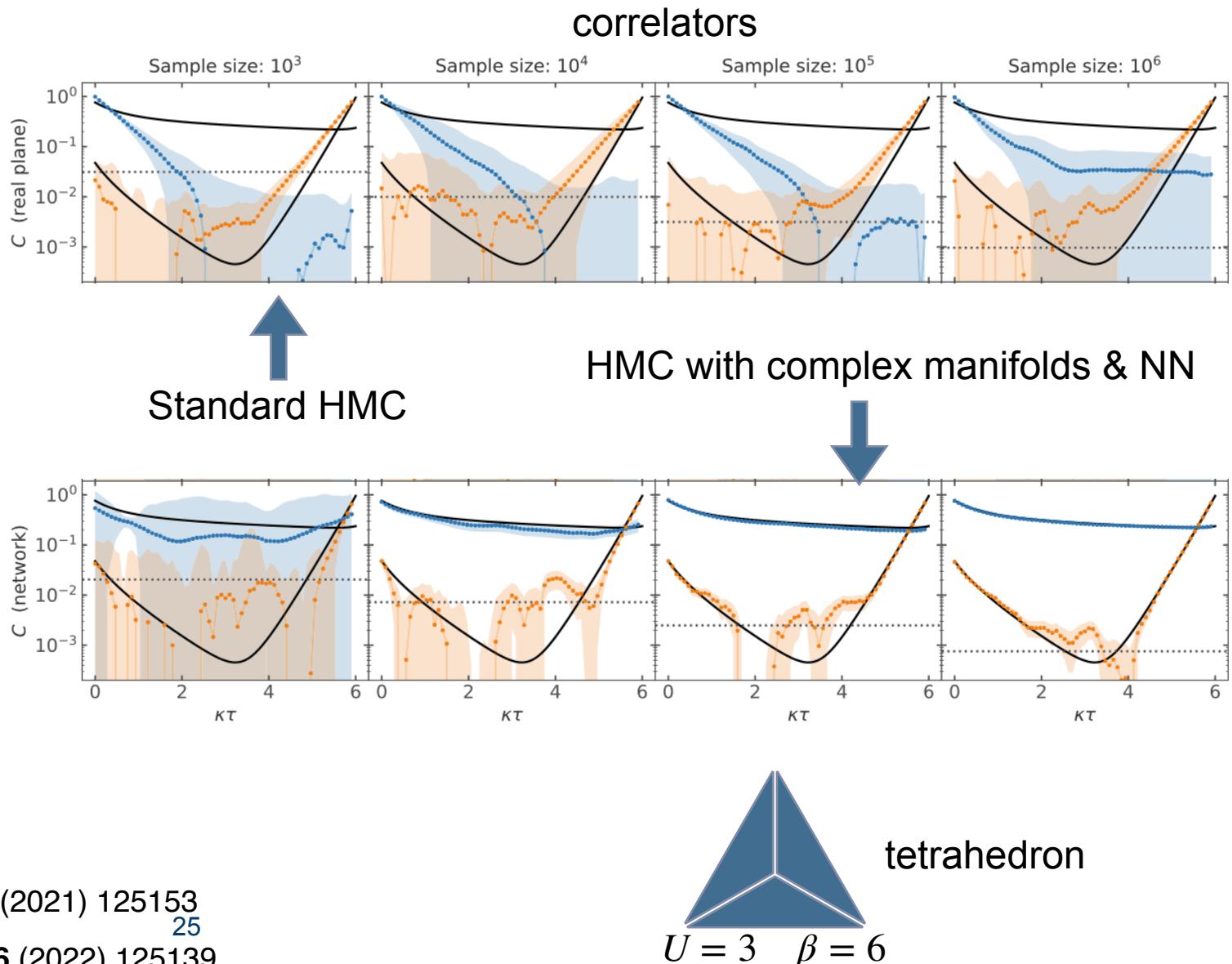
Bound three-body (trion) state
in doped systems



LOW-D SYSTEMS ARE PERFECT TESTBEDS FOR NOVEL ALGORITHMS

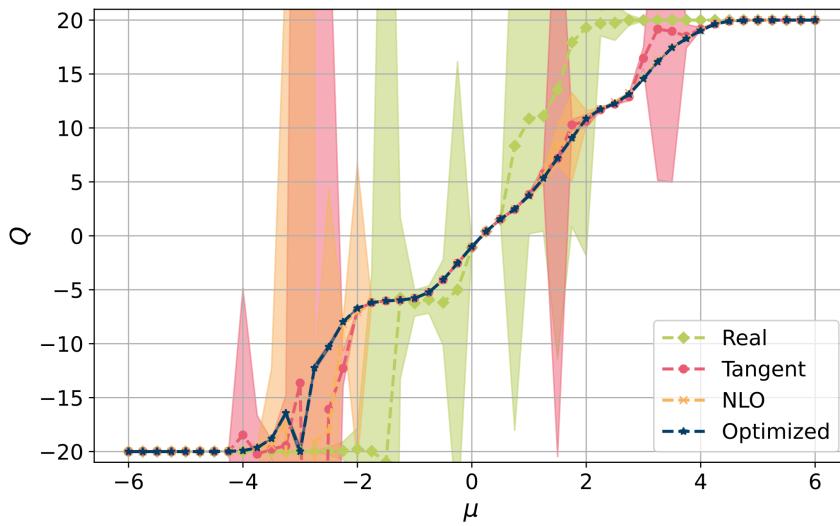
Tackling the sign problem

- Stochastic simulations at finite chemical potential
 - Suffer from numerical sign problem
 - Similar situation to LQCD
- Deform path integral contour integral into the complex plane
 - Manifolds comprising Lefschetz thimbles have significantly reduced sign problem
- Test Machine Learning (ML) algorithms to learn these manifolds and alleviate sign problem

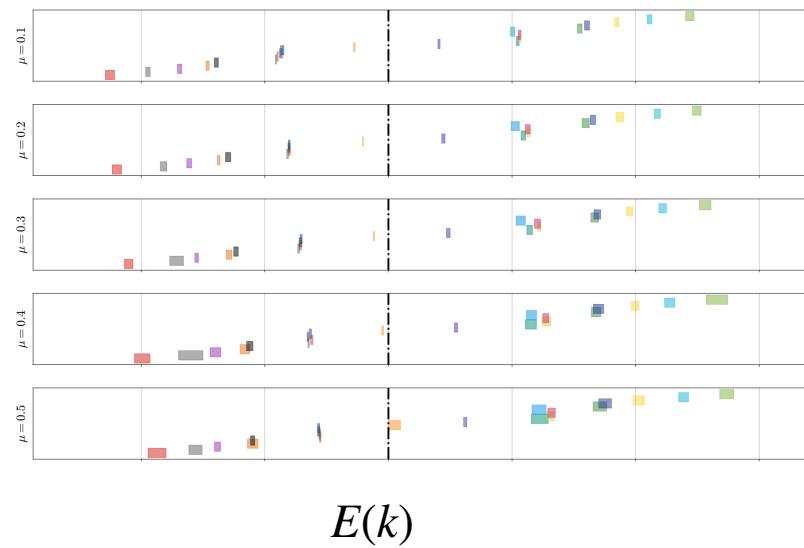
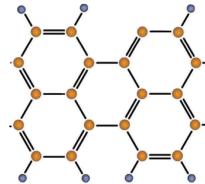


WE CAN NOW PROBE SYSTEMS NOT AVAILABLE TO US BEFORE

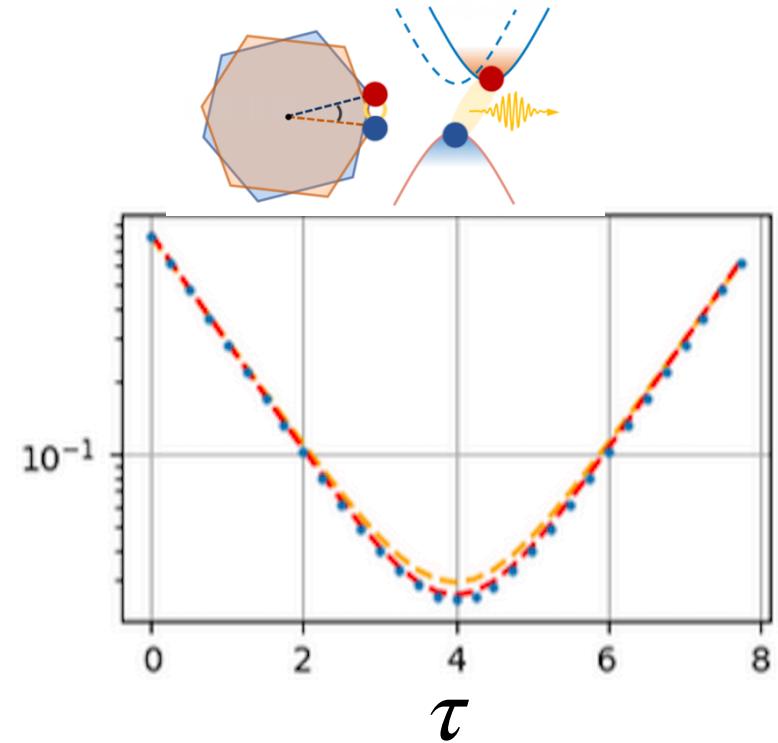
Making predictions . . .



Global charge Q of C_{20} fullerene
as a function of doping μ

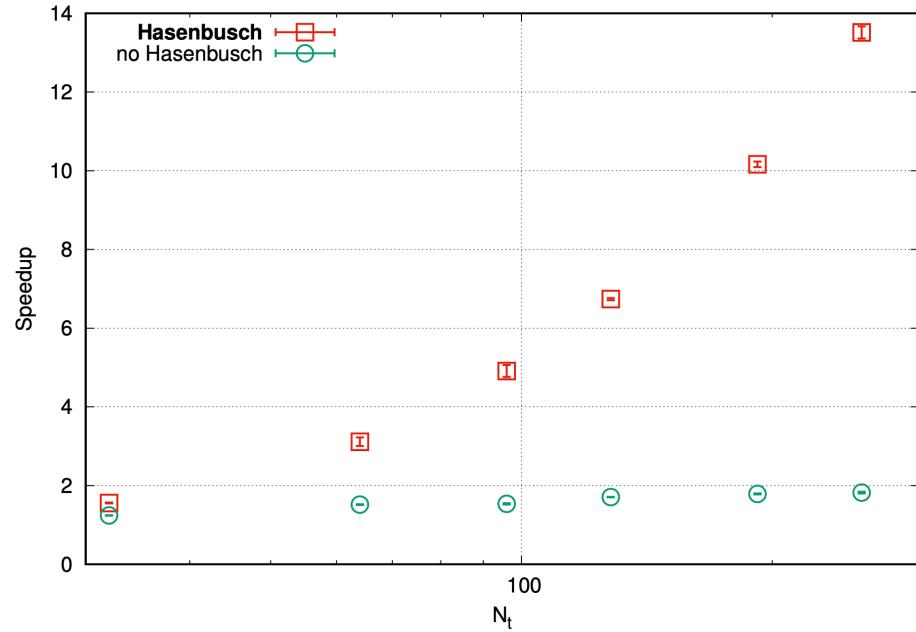


Spectrum of perylene as a
function of doping μ



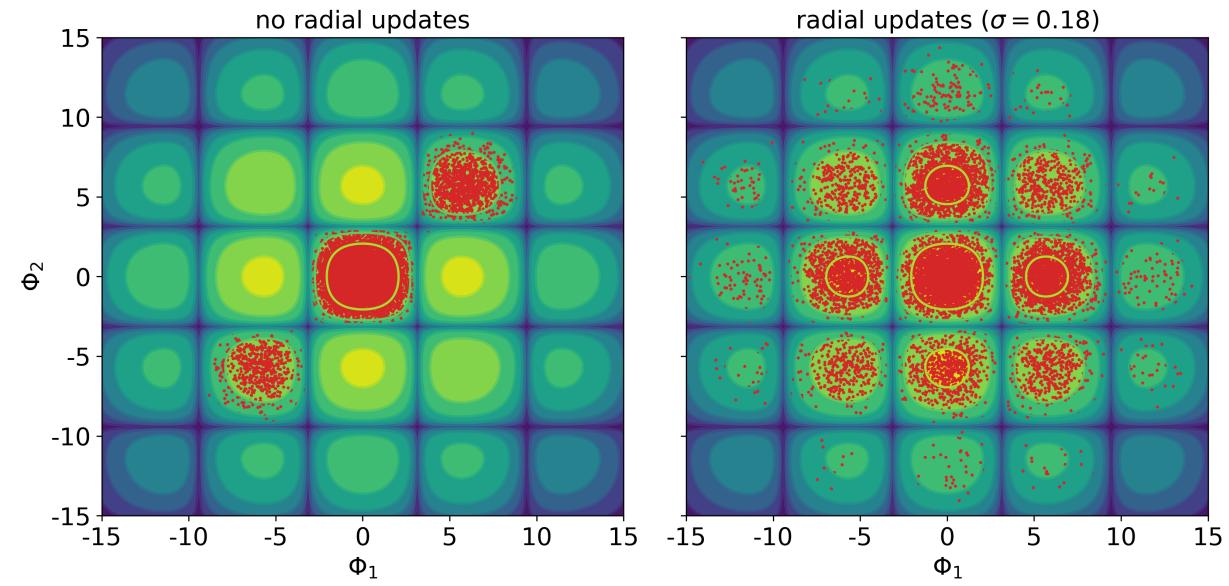
Correlators corresponding to exciton
(particle/hole) excitations

OTHER EXAMPLES OF ALGORITHMIC ADVANCEMENTS



10x speedup using Hasenbusch
preconditioning (from LQCD)

J. Ostmeyer, **TL**, C. Urbach, et al., [[arXiv:1804.07195](https://arxiv.org/abs/1804.07195)] Comput.Phys.Commun. **236** (2019) 15-25



Circumventing ergodicity problems with,
e.g. radial updates

F. Temmen, preliminary

J.-L. Wynen, **TL**, et al., [[arXiv:1812.09268](https://arxiv.org/abs/1812.09268)] Phys.Rev. **B100** (2019) 075141

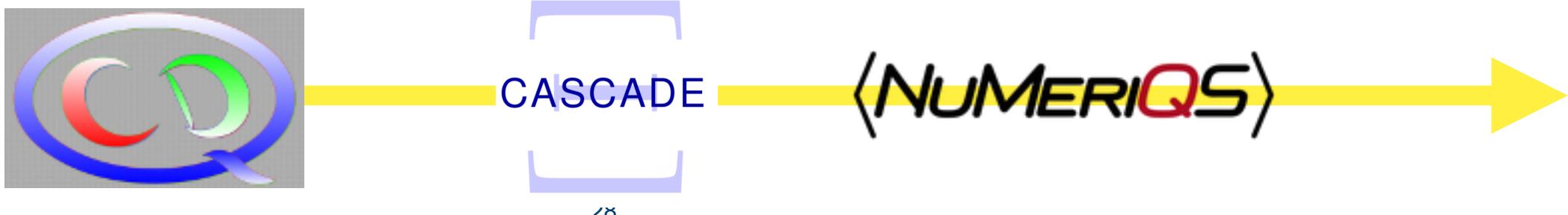
FAZIT

- Low-D materials offer fascinating novel phenomena, but require non-perturbative techniques due to strong correlation effects
- EFT methods applicable
 - Symmetries are well established
 - identification of low-energy degrees of freedom
 - separation of scales (energy gap to bulk states)
- Also great testbed for algorithmic testing and development, which already is leading to calculations in novel phase spaces

FAZIT

- Low-D materials offer fascinating novel phenomena, but require non-perturbative techniques due to strong correlation effects
- EFT methods applicable
 - Symmetries are well established
 - identification of low-energy degrees of freedom
 - separation of scales (energy gap to bulk states)
- Also great testbed for algorithmic testing and development, which already is leading to calculations in novel phase spaces

My perspectives on “Life after the CRC 110”



FAZIT

- Low-D materials offer fascinating novel phenomena, but require non-perturbative techniques due to strong correlation effects
- EFT methods applicable
 - Symmetries are well established
 - identification of low-energy degrees of freedom
 - separation of scales (energy gap to bulk states)
- Also great testbed for algorithmic testing and development, which already is leading to calculations in novel phase spaces

My perspectives on “Life after the CRC 110”



⟨NUMERIQS⟩

