Topological excitations in Hermitian and non-Hermitian interacting quantum many-body matter with tensor-network Chebyshev algorithms

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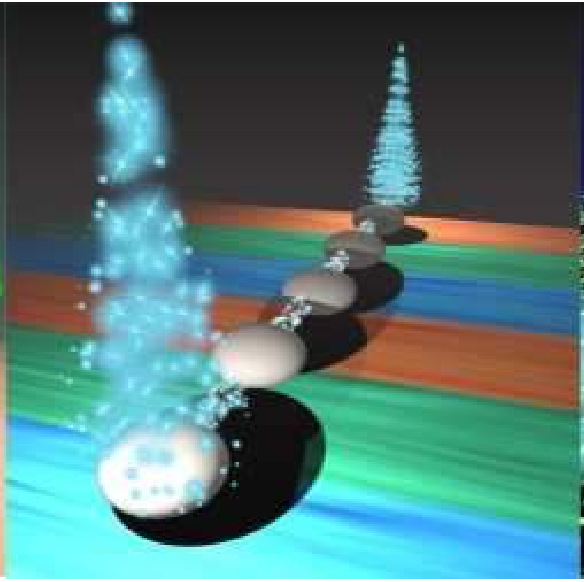
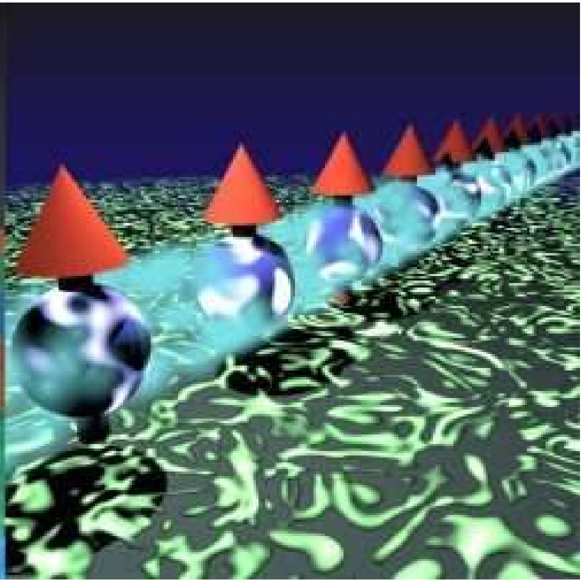
Phys. Rev. Research 3, 013095 (2021)



Phys. Rev. Research 1, 033009 (2019)
Phys. Rev. Research 2, 023347 (2020)

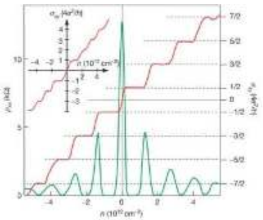


Phys. Rev. Research 4, L012006 (2022)
arXiv:2208.06425 (2022)

TQN Group Meeting Seminar, November 21st 2022

Topological matter

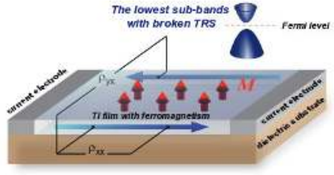
Quantum Hall effect



graphene

Nature 438, 197-200 (2005)

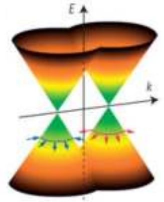
Quantum Anomalous Hall effect



Cr-doped $(Bi,Sb)_2Te_3$

Science 340.6129 (2013): 167-170

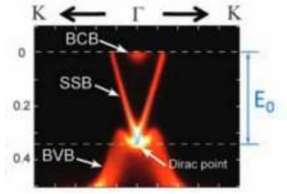
Weyl semimetal



TaAs

Nature Physics 11, 724–727 (2015)

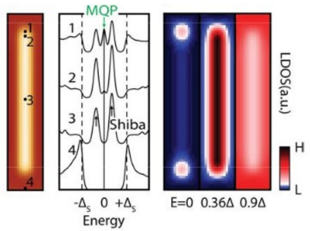
Quantum Spin Hall effect



Bi_2Se_3

Science 325.5937 (2009): 178-181

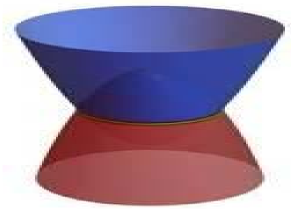
Topological superconductor



Fe@Pb

Science 346.6209 (2014): 602-607

Nodal line semimetals



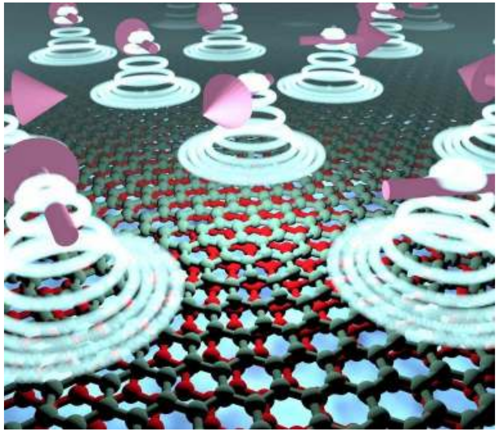
Mg_3Bi_2

Advanced Science 6.4 (2019): 1800897

All these states are described by effective single-particle Hamiltonians

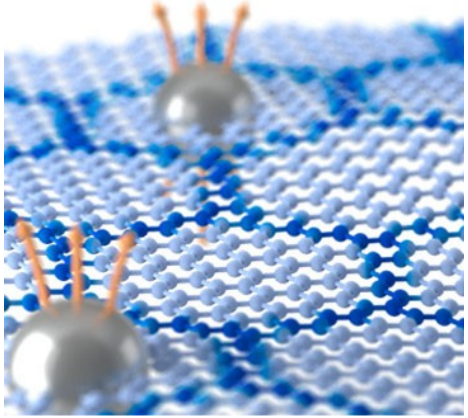
Many-body quantum matter

Quantum spin liquids



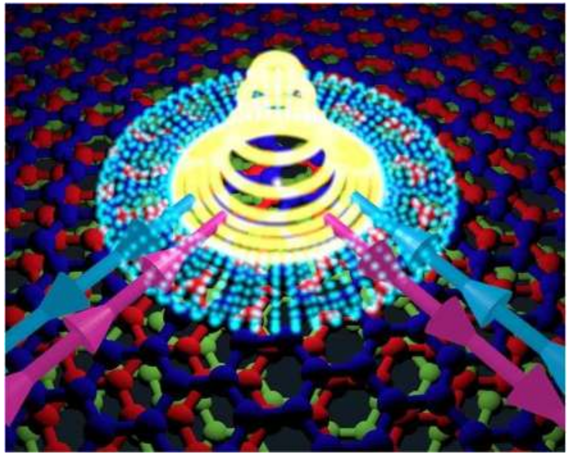
Reports on Progress in Physics 80.1 (2016): 016502.

Fractional Chern insulators



Rev. Mod. Phys. 71, S298 (1999)

Parafermions



Annual Review of Condensed Matter Physics 7, 119-139 (2016)

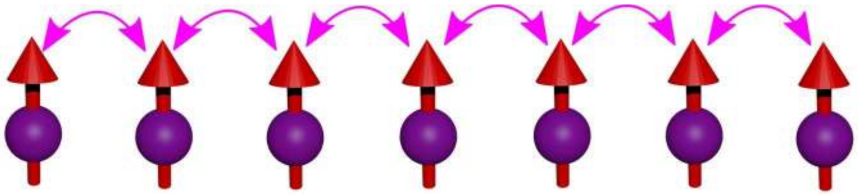
Many-body quantum matter represents an exciting critically open challenge

The problem of dimensionality

In a many-body problem, the size of our vectors grows as

$$2^L$$ where L is the number of sites

$$\mathcal{H} = \sum_{\langle ij \rangle} J \vec{S}_i \cdot \vec{S}_j$$



For a single-particle tight binding problem, we can reach up to 10^8 sites in a laptop

For a many-problem, we cannot even store states for systems bigger than $L = 30$ sites

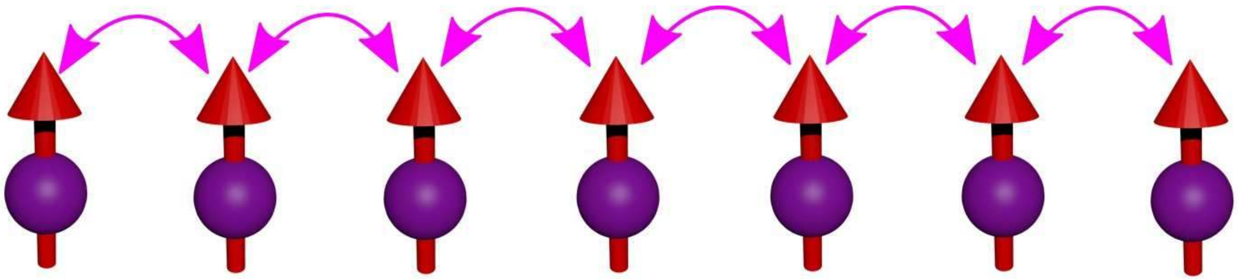
$$2^{30} \sim 10^9$$

How can be compute dynamical properties if we cannot even store the states?

Many-body dynamical correlators

One dimensional Heisenberg Hamiltonian

$$\mathcal{H} = \sum_{\langle ij \rangle} J \vec{S}_i \cdot \vec{S}_j$$



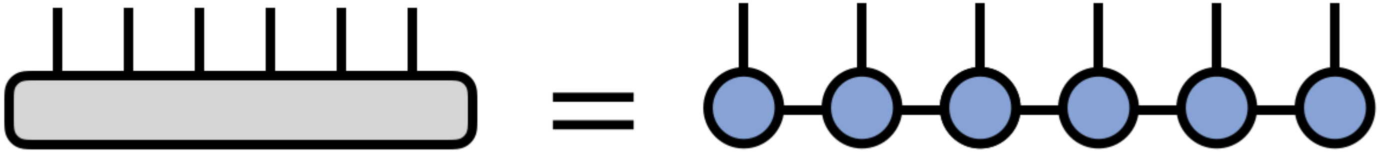
We want to compute the dynamical correlator

$$\mathcal{S}(N,\omega) = \langle GS | S^z_N \delta(\omega - \mathcal{H} + E_0) S^z_N | GS \rangle$$

State compression with tensor-networks

Given a many-body wavefunction, we can parametrice the components as

$$|\Psi\rangle = \sum_{\{s\}} \mathrm{Tr}\left[A_1^{(s_1)} A_2^{(s_2)} \cdots A_N^{(s_N)}\right] |s_1 s_2 \ldots s_N\rangle$$



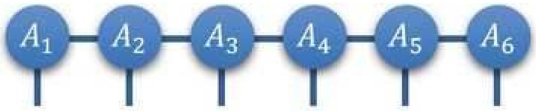
Matrix product state

The previous representation allows drastically reducing the memory required to store a state

Annals of Physics 326, 96 (2011)

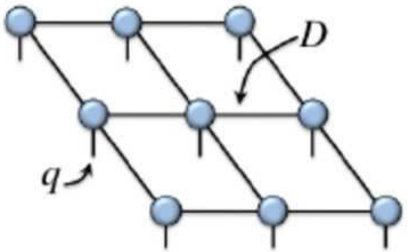
Many-body state compression

Matrix-product states



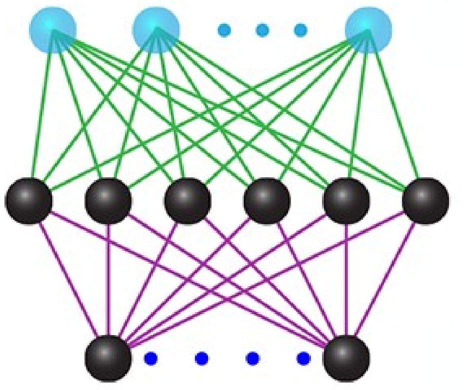
Phys. Rev. Lett. 69, 2863 (1992)

Projected entangled pair-states



Annals of Physics 326, 96 (2011)

Neural-network quantum states



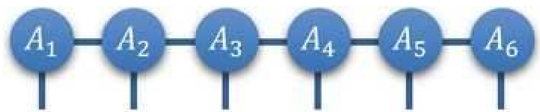
Science 355.6325 (2017): 602-606.

Compressed many-body states allow using kernel-polynomial methods for many-body systems

The kernel-polynomial tensor-network algorithm

Take a many-body Hamiltonian $$\mathcal{H} = \sum_{\langle ij \rangle} J \vec{S}_i \cdot \vec{S}_j$$

Obtain a tensor-network representation of the many-body ground state

$$|GS\rangle =$$ 

And apply the kernel polynomial algorithm in the compressed representation

$$\bar{\chi}(\omega) = \langle \mathrm{GS}|S_N^z \delta(\omega - \bar{H}) S_N^z|\mathrm{GS}\rangle$$

$$\bar{\chi}(\omega) = \frac{1}{\pi\sqrt{1-\omega^2}}\left[\mu_0 + 2\sum_{l=1}^{N_P} \mu_l T_l(\omega)\right]$$

$$\mu_l = \langle \mathrm{GS}|S_N^z T_l(\bar{H}) S_N^z|\mathrm{GS}\rangle$$

$$\mu_l = \langle \mathrm{GS}|S_N^z|w_l\rangle$$

$$|w_0\rangle = S_N^z|\mathrm{GS}\rangle,$$

$$|w_1\rangle = \bar{H}|w_0\rangle,$$

$$|w_{l+1}\rangle = 2\bar{H}|w_l\rangle - |w_{l-1}\rangle,$$

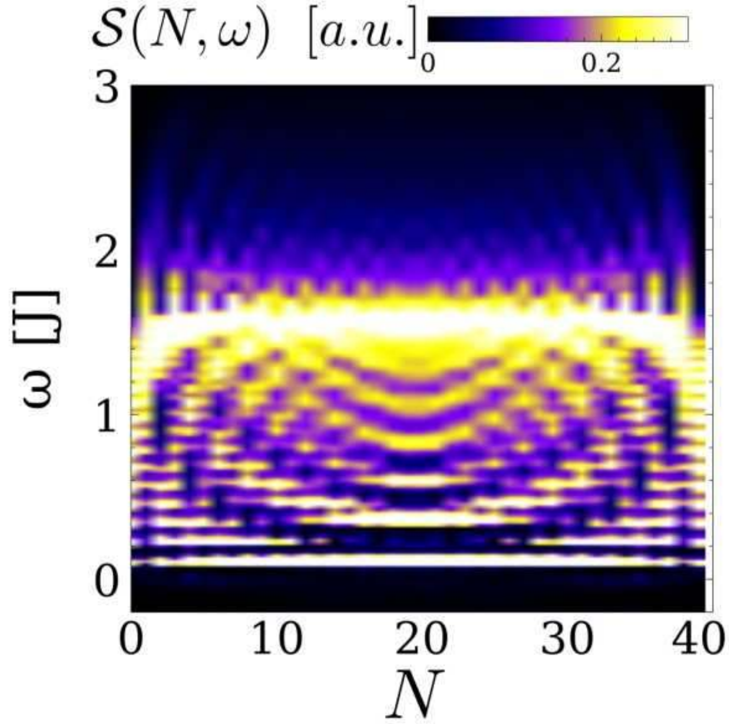
Rev. Mod. Phys. 78, 275 (2006)

Phys. Rev. Research 1, 033009 (2019)

Open-source implementation in *https://github.com/joselado/dmrgpy*

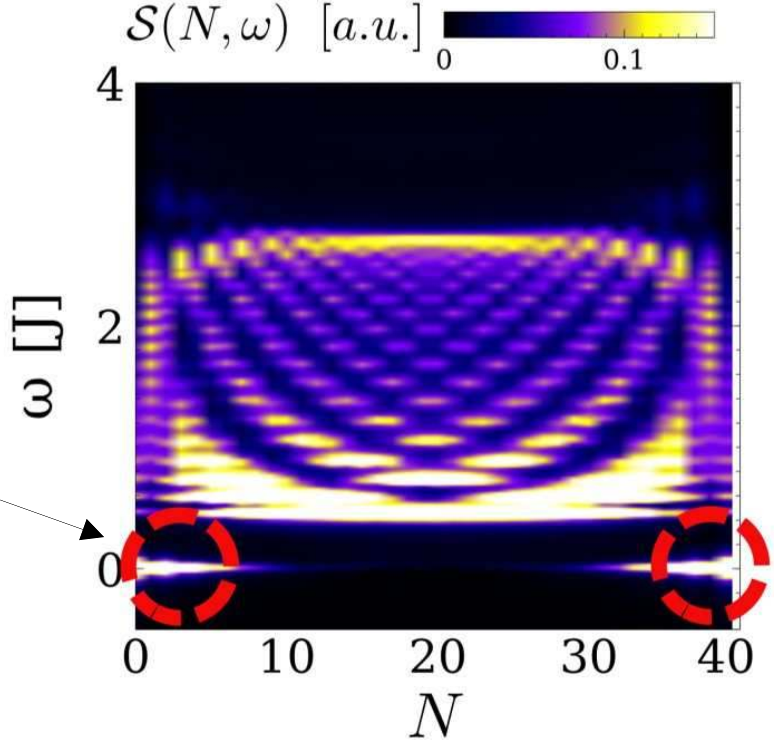
Dynamical structure factor of a Heisenberg model

S=1/2 chain



S=1 chain

Edge modes



Behind the scenes

Many-body parafermions

Vilja Kaskela

Phys. Rev. Research 3, 013095 (2021)

Without a single-particle counterpart

Quasiperiodic many-body topology

Malte Rösner

Oded Zilberberg

Phys. Rev. Research 3, 013265 (2021)
Phys. Rev. Research 1, 033009 (2019)

Driven by quasiperiodicity

Non-Hermitian many-body topology

Timo Hyart

Fei Song

Guangze Chen

Phys. Rev. Research 4, L012006 (2022)
arXiv:2208.06425 (2022)

Driven by losses

Topological excitations in parafermion chains

Majorana fermions and parafermions

The Z_n parafermion algebra is given by

$$z = e^{2\pi i/n}$$

$$\chi_j \psi_k = z \psi_k \chi_j, \quad \chi_j \chi_k = z \chi_k \chi_j, \quad \psi_j \psi_k = z \psi_k \psi_j$$

For n=2 we have conventional Majorana fermions

For n>2 we have Z_n parafermions

<u>For n>2, quadratic models cannot be mapped to a single particle Hamiltonian</u>

n>3 Z_n parafermion models are purely many-body

The general parafermion model

The simplest model for coupled parafermions is

$$\mathcal{H} = if \sum_n \chi_n^\dagger \psi_n + i\theta \sum_n \psi_n^\dagger \chi_{n+1} + \mathrm{H.c.},$$

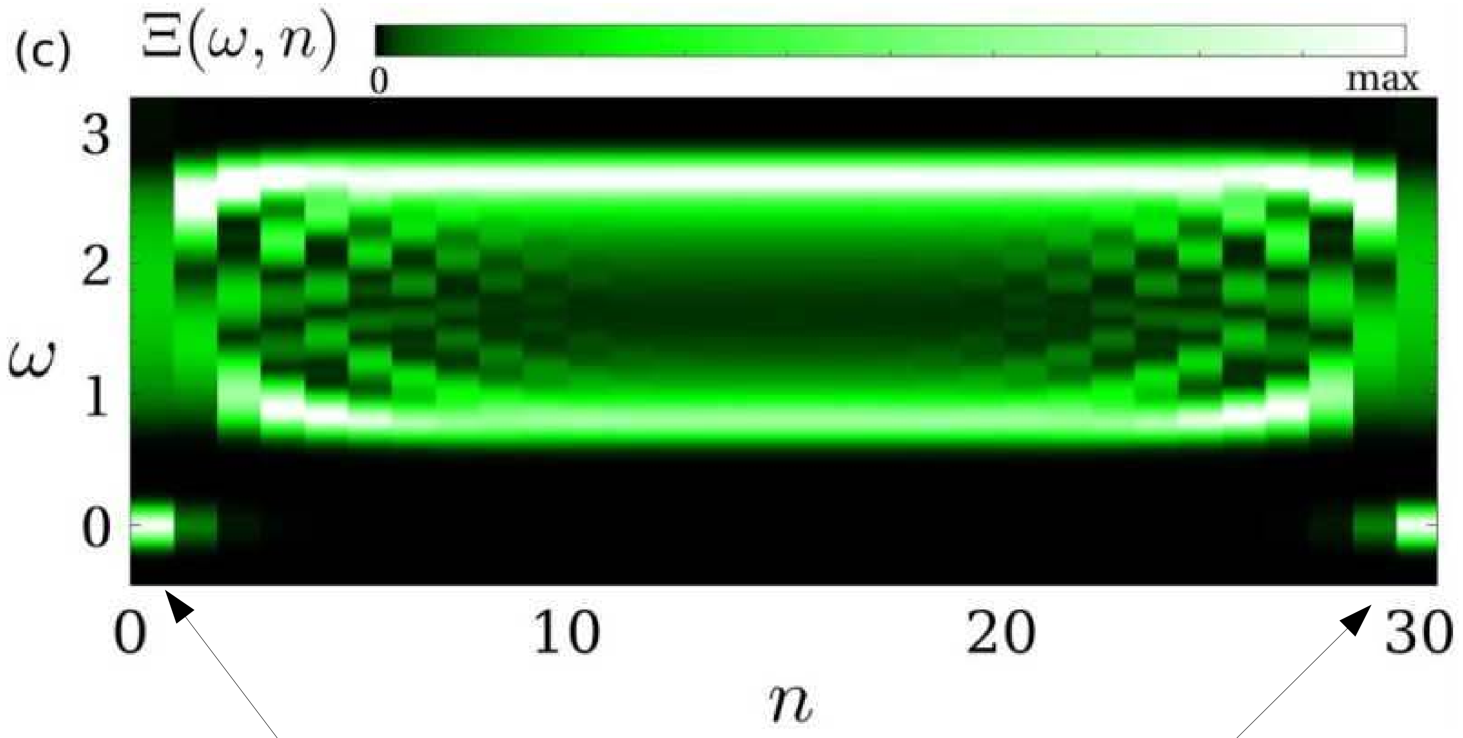
with $\chi_j \psi_k = z \psi_k \chi_j, \quad \chi_j \chi_k = z \chi_k \chi_j, \quad \psi_j \psi_k = z \psi_k \psi_j$

(for n=2, this is just the Kitaev model for topological superconductors)

We will compute the dynamical excitations (parafermion version of density of states)

$$\Xi(\omega, n) = \langle \mathrm{GS} | \chi_n^\dagger \delta(\omega - \mathcal{H} + E_{\mathrm{GS}}) \psi_n | \mathrm{GS} \rangle.$$

Edge modes in parafermion models

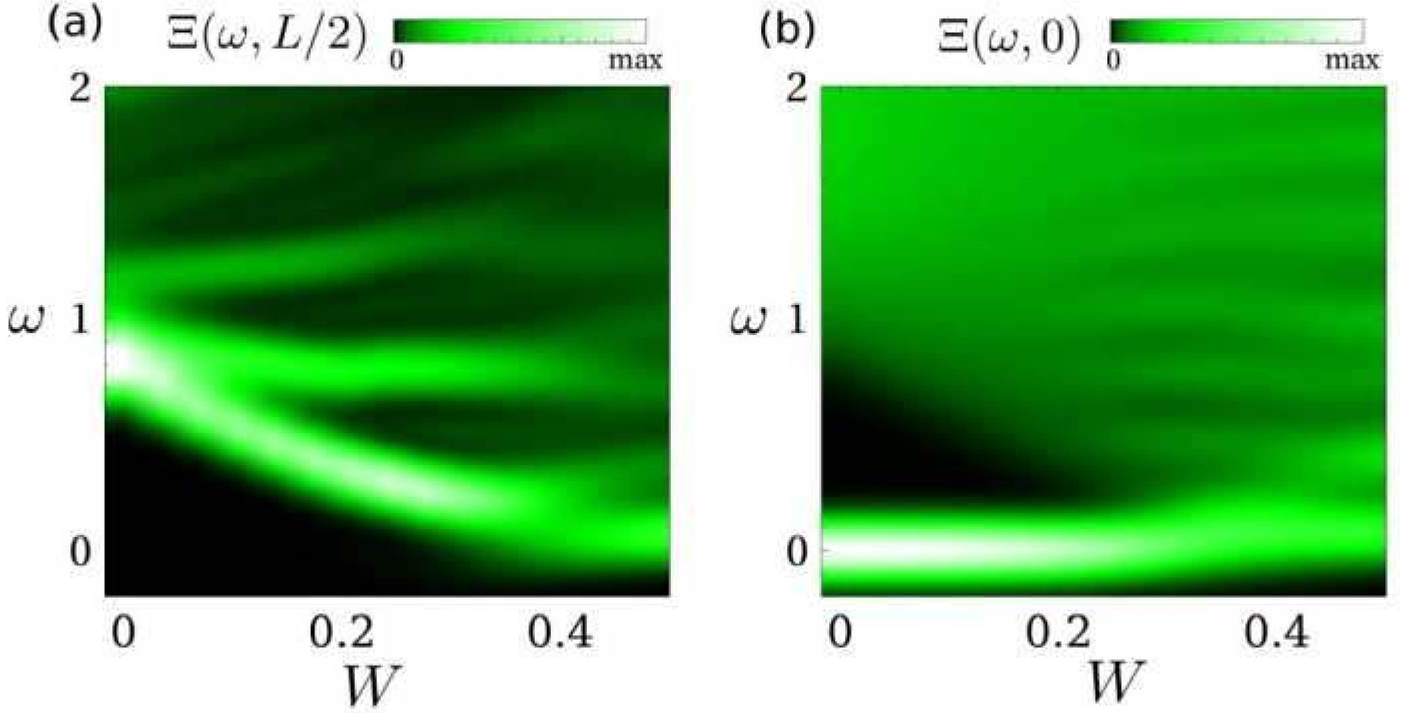


Topological parafermion zero modes

Four-parafermion interactions

Bulk **Edge**

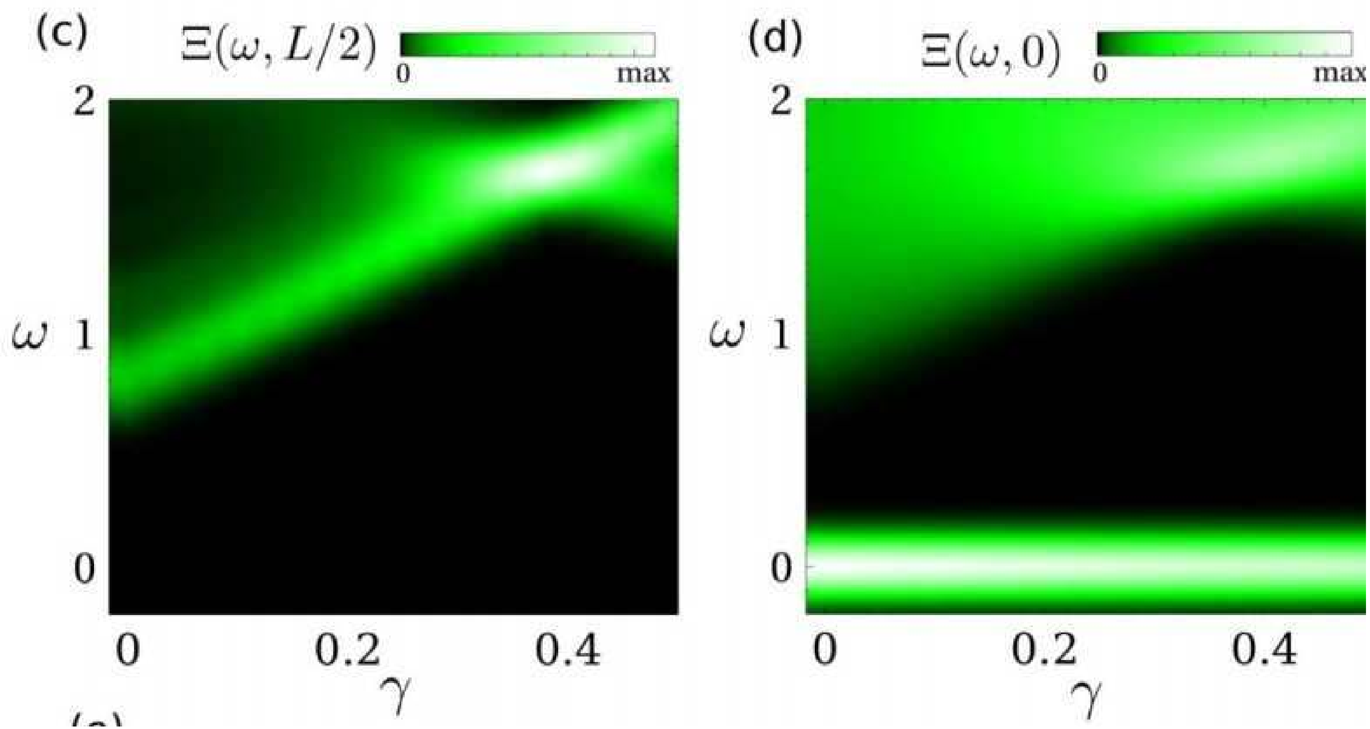
$$W \sum_n \psi_n^\dagger \chi_n \psi_{n+1}^\dagger \chi_{n+1}$$



Zero modes survive in the presence of perturbations

Next-to-nearest neighbor coupling

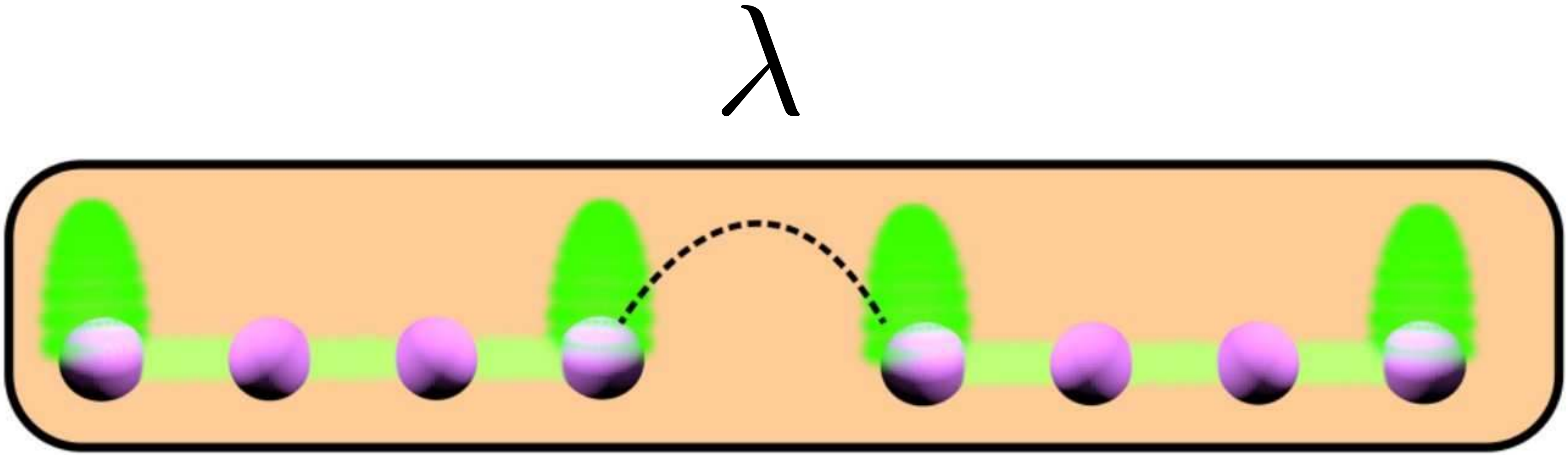
Bulk **Edge**



$$-\gamma \sum_{n} \psi_n^{\dagger} \chi_{n+2}$$

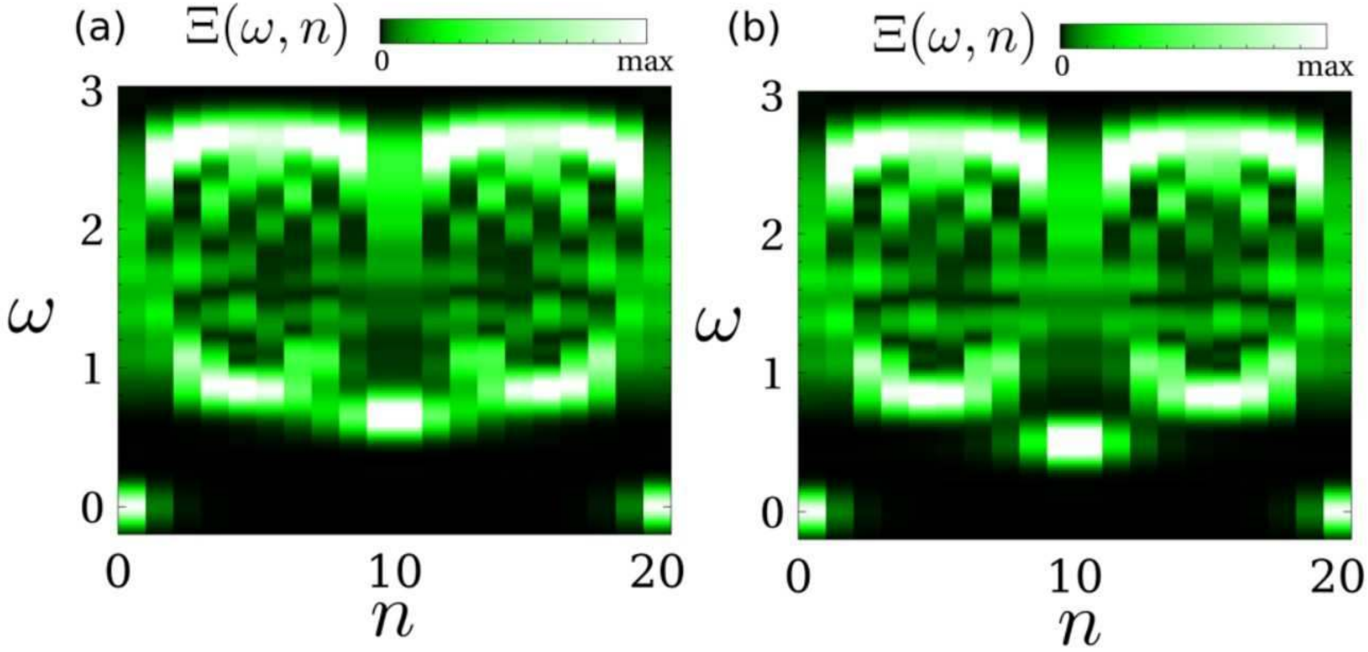
Zero modes survive in the presence of perturbations

Weakly coupled parafermions



Weakly coupled parafermions

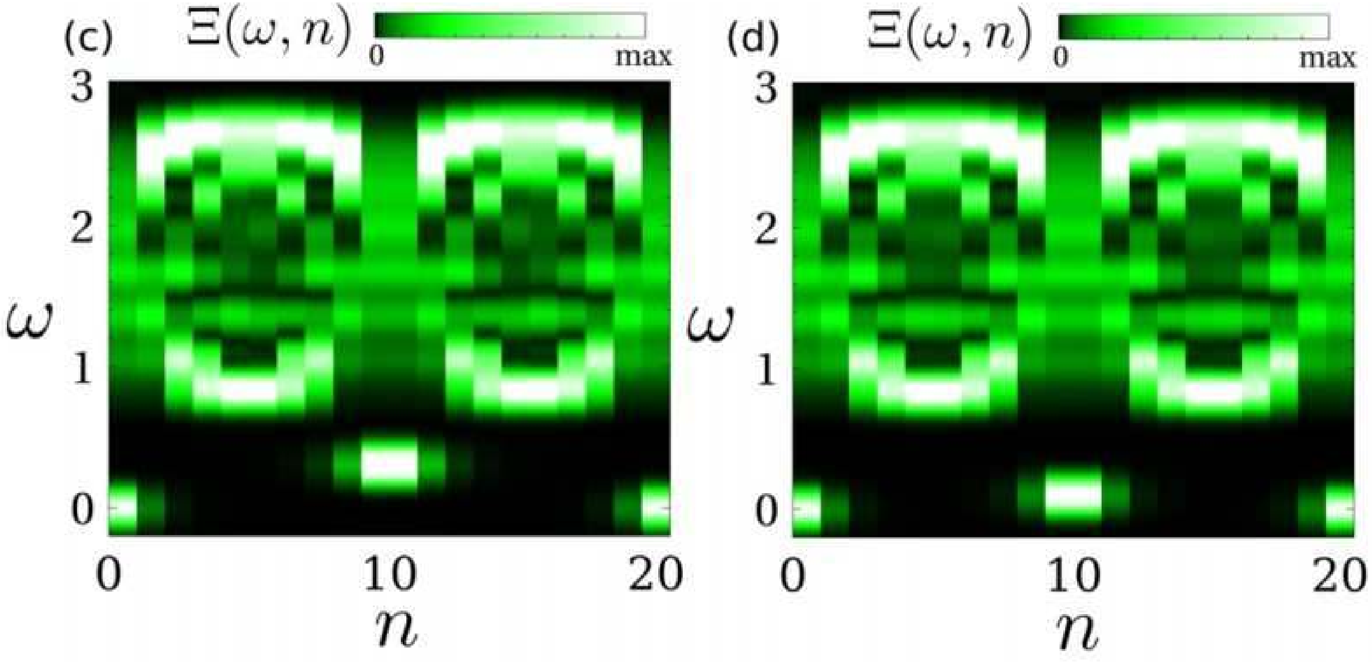
$\lambda = 0.7$ $\lambda = 0.5$



As the chain is decoupled, in-gap parafermion modes appear

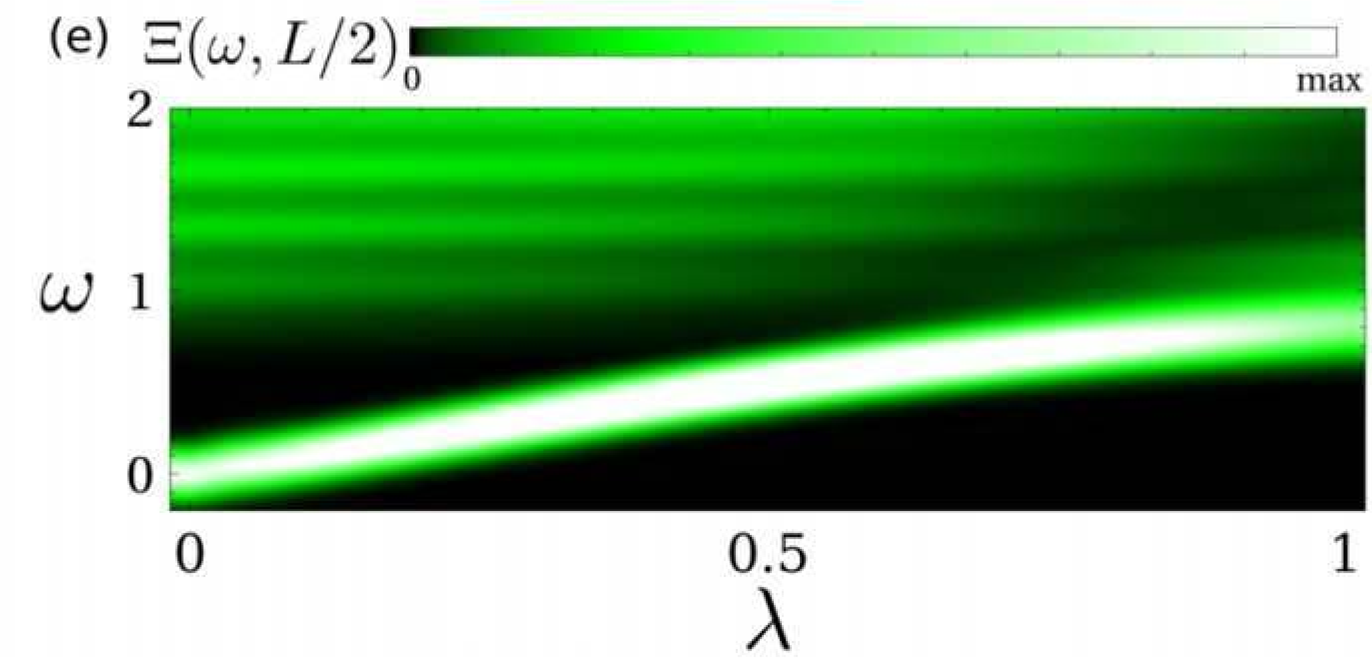
Weakly coupled parafermions

$\lambda = 0.3$ $\lambda = 0.1$



As the chain is decoupled, in-gap parafermion modes appear

Weakly coupled parafermions

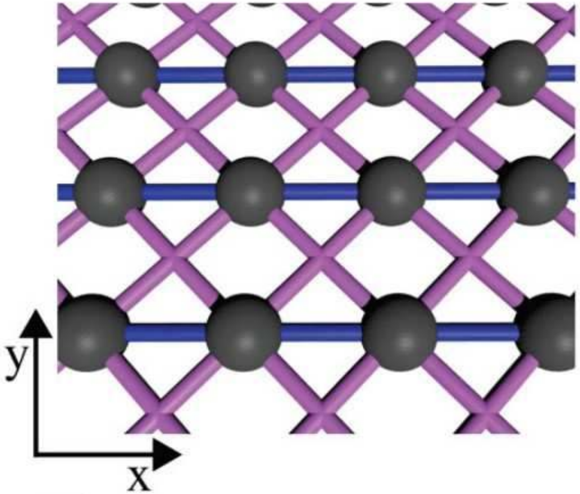


The energy of the in-gap parafermion is controlled by the coupling

Coulomb modulated topology

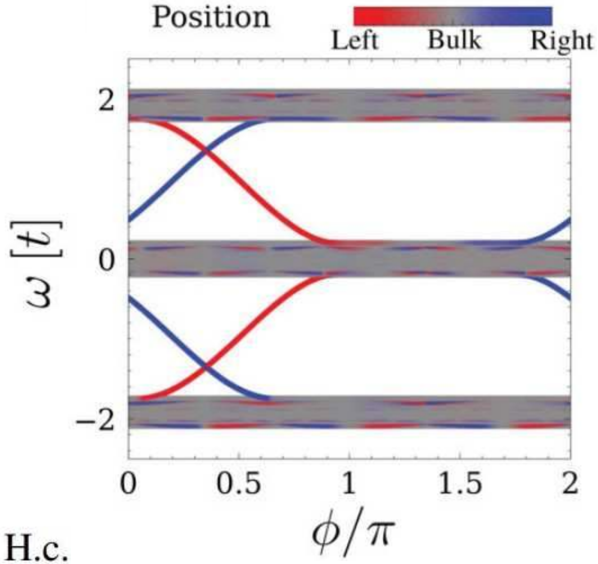
Quasiperiodic topology

Quantum Hall in a
two-dimensional lattice



$\sim$

Spectrum of the associated
quasiperiodic Hamiltonian



$$H = t \sum_N [1 + \lambda \cos(\alpha N + \phi)] c_N^\dagger c_{N+1} + \mathrm{H.c.}$$

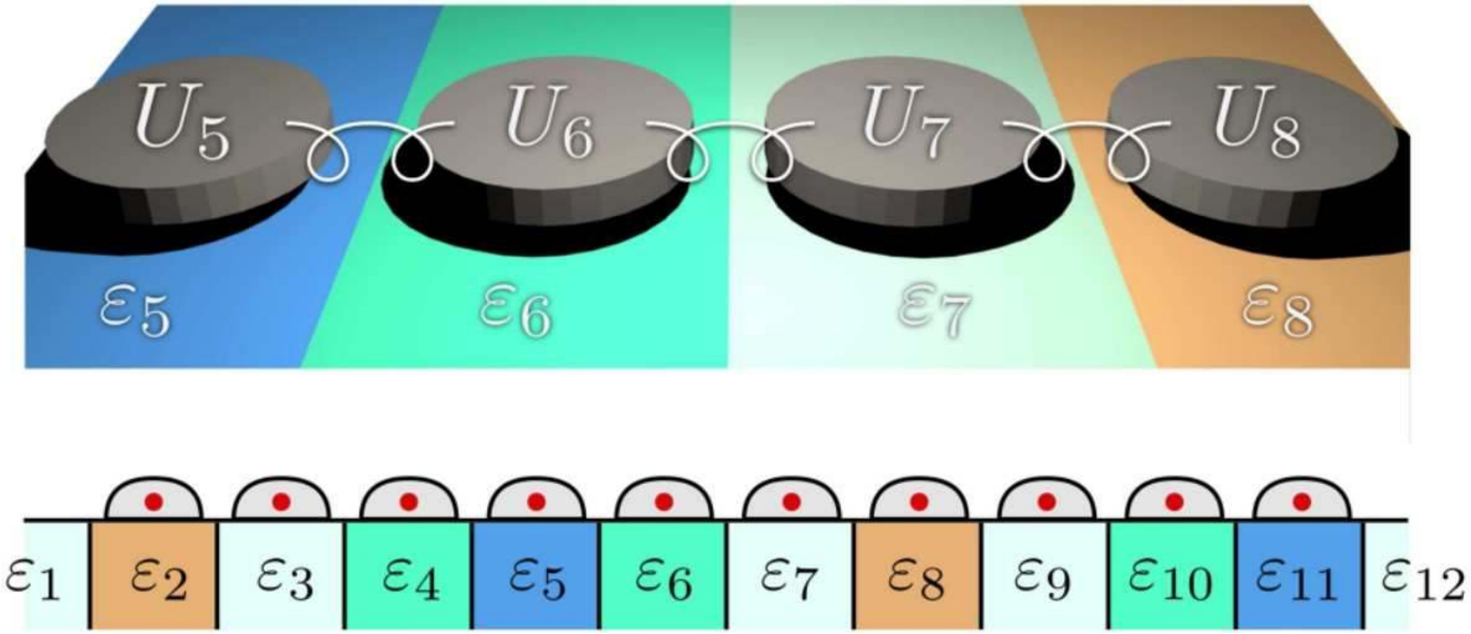
1D quasiperiodic models can be mapped to 2D quantum Hall states

This mapping is only valid in the non-interacting limit

Phys. Rev. Lett. 109, 116404 (2012)

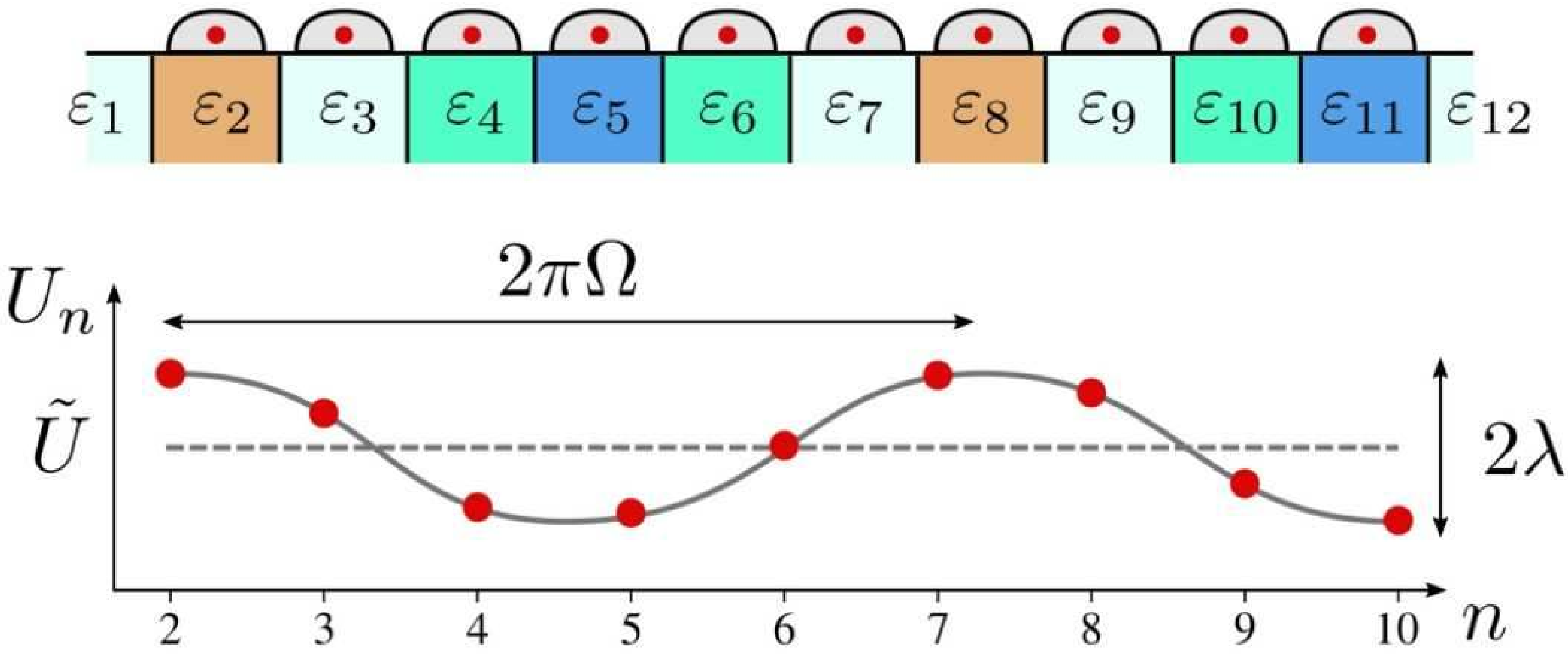
Many-body quasiperiodic interactions

Substrate engineering allow creating spatially dependent interactions



$$H = \sum_{n,s} t\, c^\dagger_{n,s} c_{n+1,s} + \sum_n U_n c^\dagger_{n,\uparrow} c_{n,\uparrow} c^\dagger_{n,\downarrow} c_{n,\downarrow} + h.c. \qquad U_n = \tilde{U}[1 + \lambda \cos(\Omega n + \phi)]$$

Many-body quasiperiodic interactions



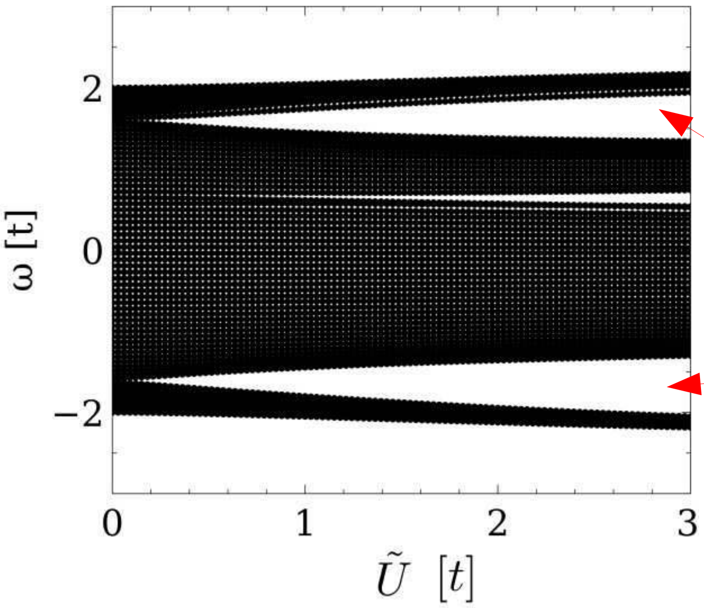
$$H = \sum_{n,s} t\, c^\dagger_{n,s} c_{n+1,s} + \sum_n U_n c^\dagger_{n,\uparrow} c_{n,\uparrow} c^\dagger_{n,\downarrow} c_{n,\downarrow} + h.c. \qquad U_n = \tilde{U}[1 + \lambda \cos(\Omega n + \phi)]$$

Warm-up: single particle Coulomb-engineered topology

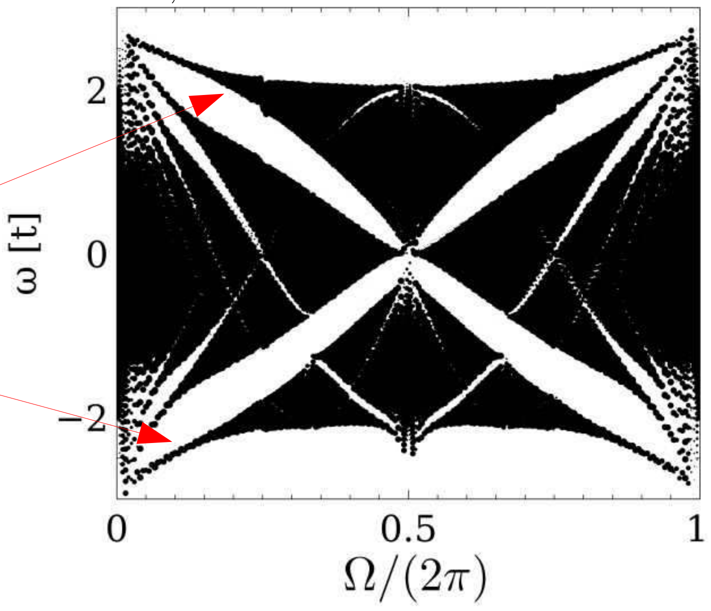
Engineered interacting model $$H = \sum_{n,s} t\, c^\dagger_{n,s} c_{n+1,s} + \sum_n U_n c^\dagger_{n,\uparrow} c_{n,\uparrow} c^\dagger_{n,\downarrow} c_{n,\downarrow} + h.c.$$

Modulated interactions $$U_n = \tilde{U}[1 + \lambda \cos(\Omega n + \phi)]$$

Solved at the Hartree-Fock level $$\sum_{s,s'} \langle \vec{\sigma}_{s,s'} c^\dagger_{n,s} c_{n,s'} \rangle = 0$$



Topological gap opening

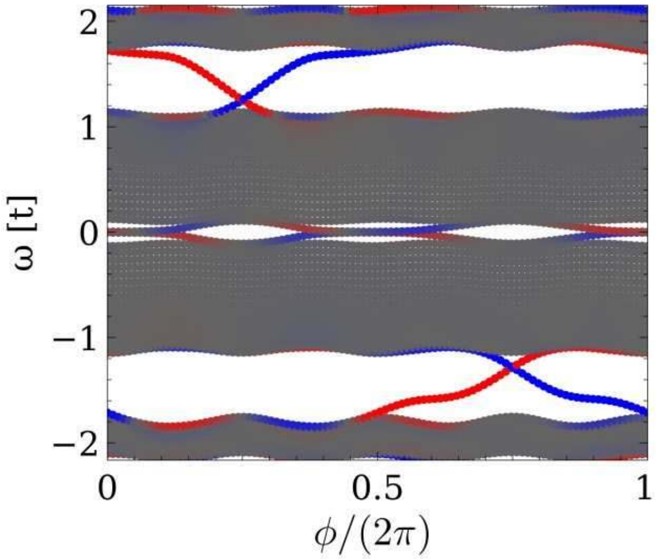


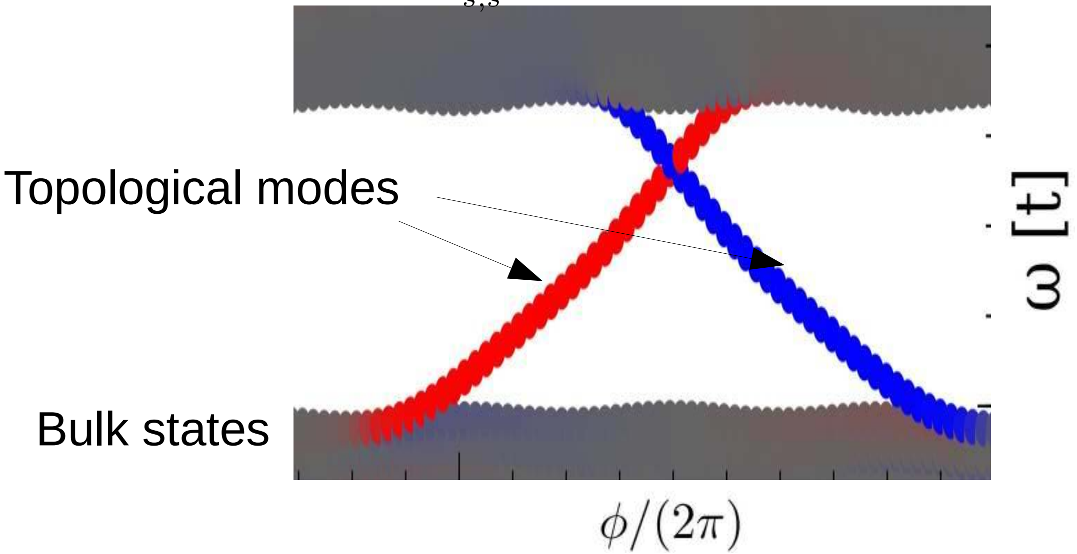
Warm-up: single particle Coulomb-engineered topology

Engineered interacting model $$H = \sum_{n,s} t\, c^\dagger_{n,s} c_{n+1,s} + \sum_n U_n c^\dagger_{n,\uparrow} c_{n,\uparrow} c^\dagger_{n,\downarrow} c_{n,\downarrow} + h.c.$$

Modulated interactions $$U_n = \tilde{U}[1 + \lambda \cos(\Omega n + \phi)]$$

Solved at the Hartree-Fock level $$\sum_{s,s'} \langle \vec{\sigma}_{s,s'} c^\dagger_{n,s} c_{n,s'} \rangle = 0$$





Modulated local interactions create topological modes

Many-body topology

Let us focus in an interacting Hamiltonian with a trivial mean-field Hamiltonian

$$H = \sum_{n,s} t\, c^\dagger_{n,s} c_{n+1,s} + \sum_n U_n \left(c^\dagger_{n,\uparrow} c_{n,\uparrow} - \frac{1}{2} \right) \left(c^\dagger_{n,\downarrow} c_{n,\downarrow} - \frac{1}{2} \right) + h.c.$$

In the many-body setting, we will look at the dynamical spin excitation spectra

$$\mathcal{S}(\omega, n) = \langle GS | S^z_n \delta(\omega - H + E_{GS}) S^z_n | GS \rangle$$

Computed with the kernel polynomial tensor network formalism

$$\mathcal{S}(\omega, n) = \frac{1}{\pi\sqrt{1-\omega^2}} [\mu_0 + 2 \sum_{k=1}^{N} \mu_k T_k(\omega)]$$

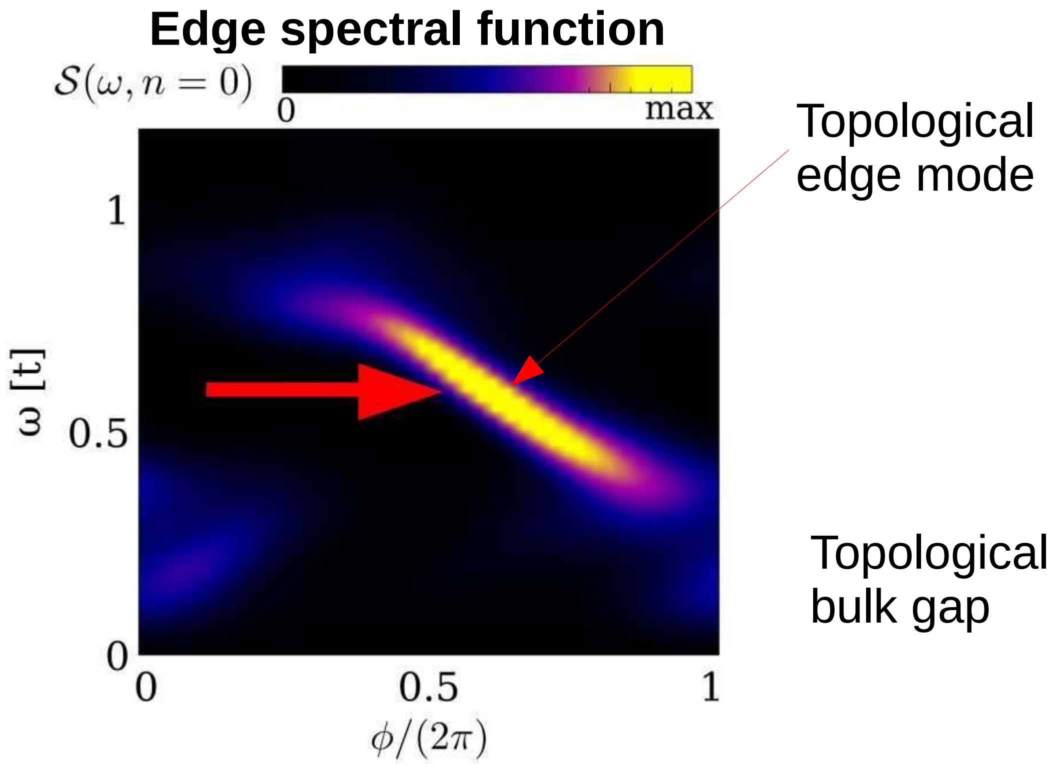
$$\mu_k = \langle GS | S^z_n T_k(H) S^z_n | GS \rangle$$

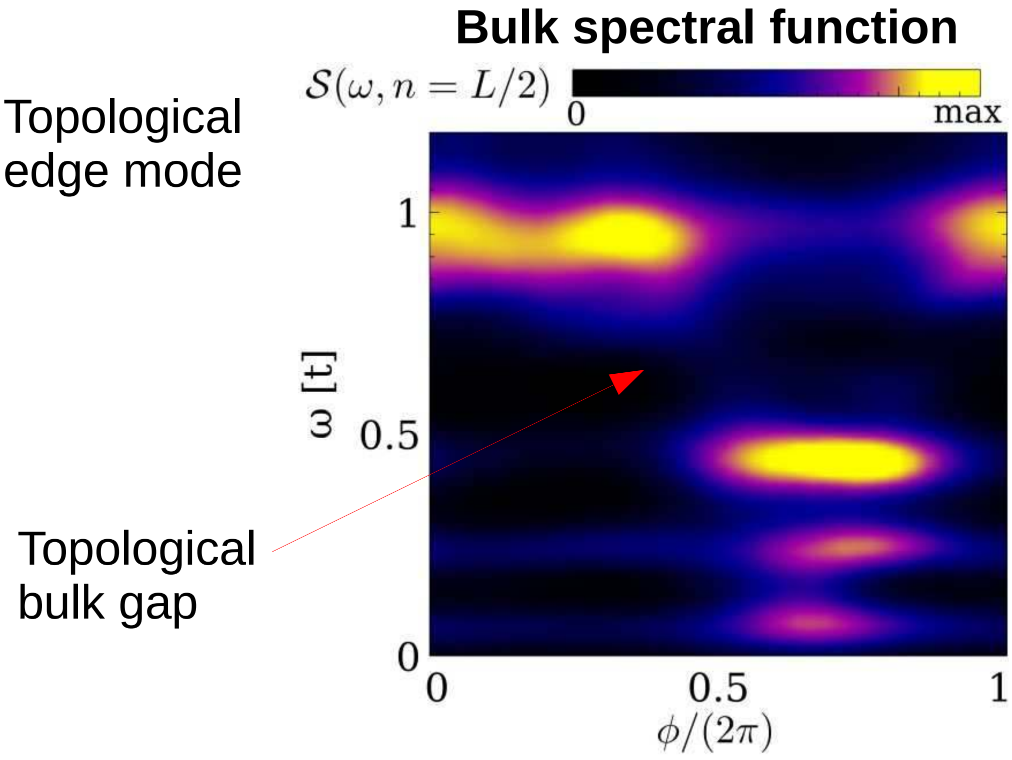
https://itensor.org/

Rev. Mod. Phys. 78, 275 (2006)

https://github.com/joselado/dmrgpy

Many-body topological modes



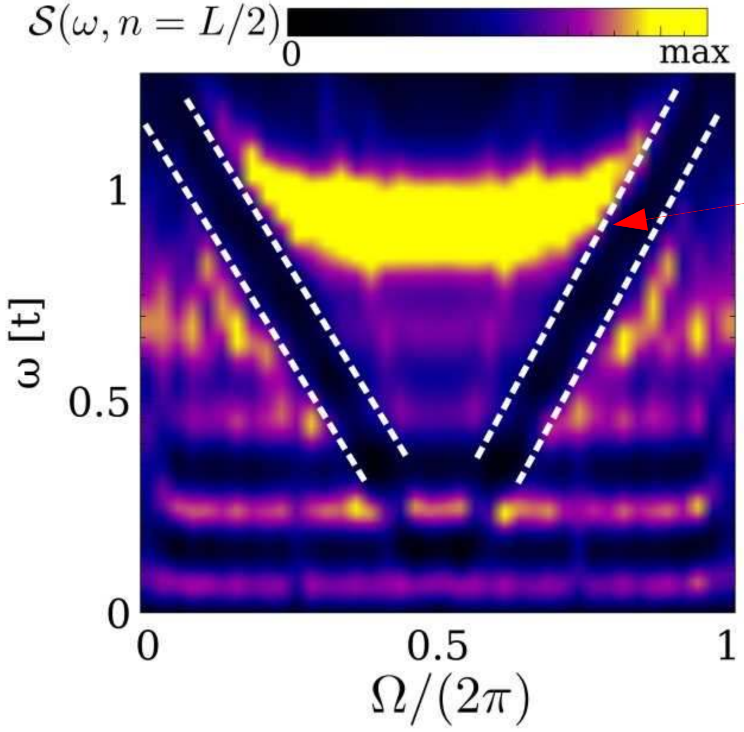


Topological modes protected by a many-body quasiperiodic Chern invariant

Phys. Rev. Research 1, 033009 (2020) *arXiv:2009.03752* *arXiv:2010.06171*

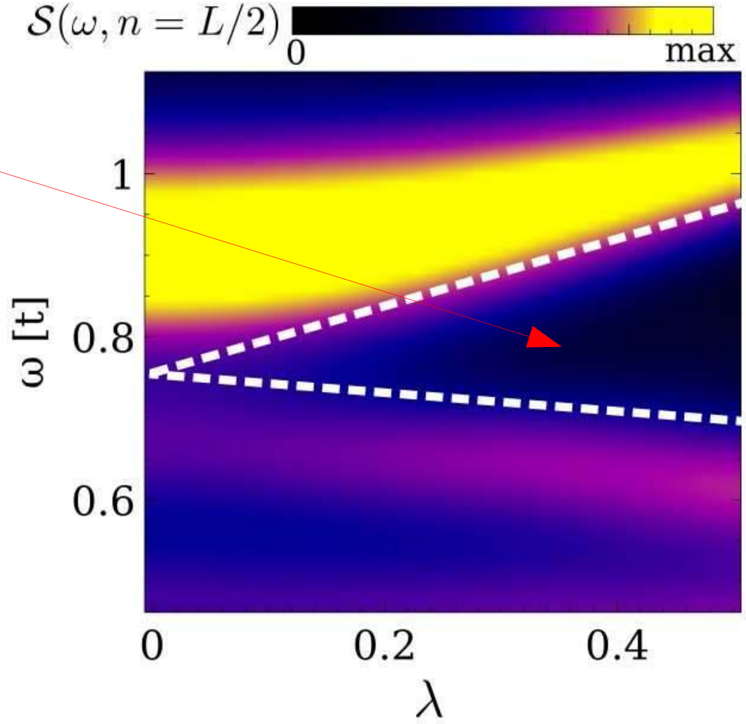
Many-body topological gaps

Bulk spectral function



Topological bulk gap

Bulk spectral function



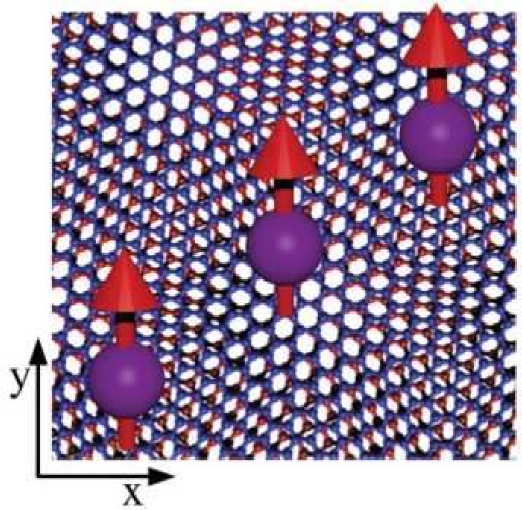
Topological gaps appear for generic modulation frequencies and strengths

Quasiperiodic spinon topology

Quasiperiodic spinon topology

Many-body spin Hamiltonians can be intrinsically quasiperiodic

For example, an atomic chain on top of a moire system

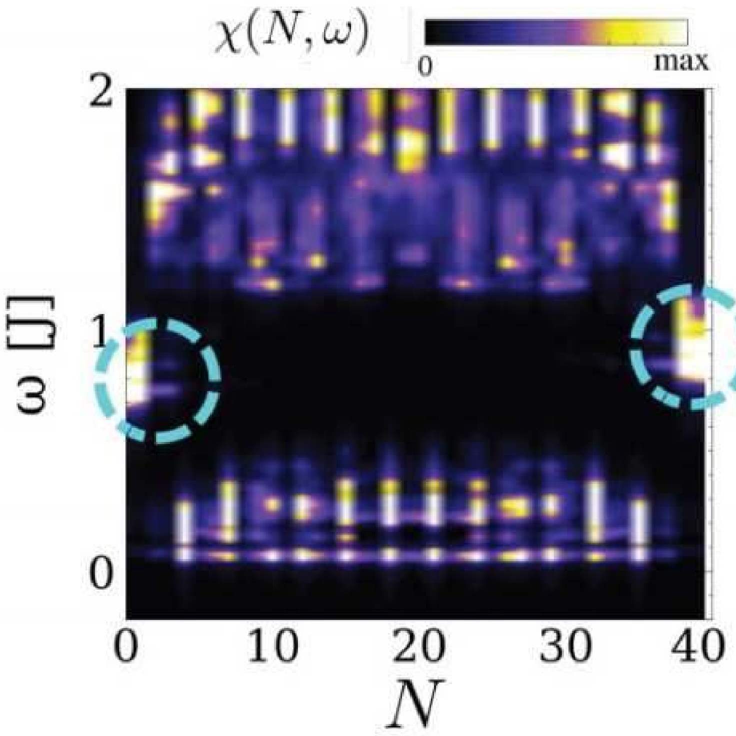


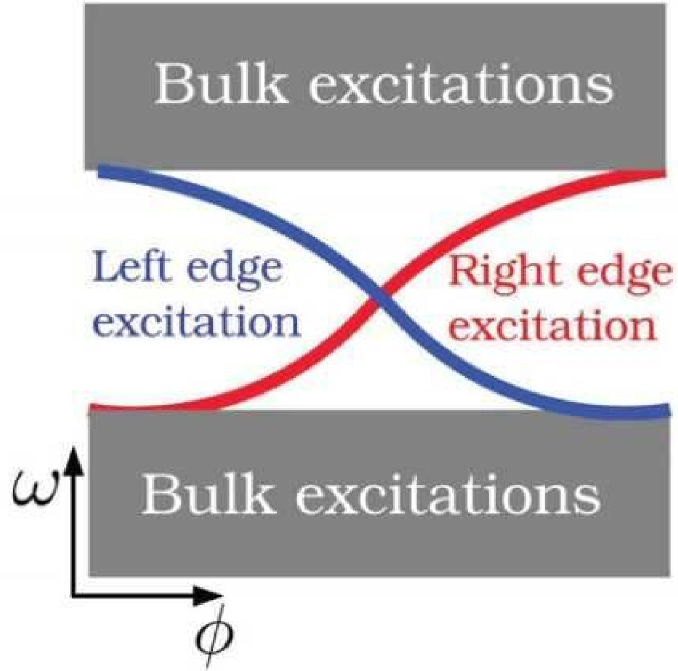
We will consider the generalized quasiperiodic Heisenberg model

$$H = J \sum_N [1 + \lambda \cos(\alpha N + \phi)] \vec{S}_N \cdot \vec{S}_{N+1}$$

with $S = 1/2, 1, 3/2, 2$

Topological quasiperiodic spinon for S=1/2

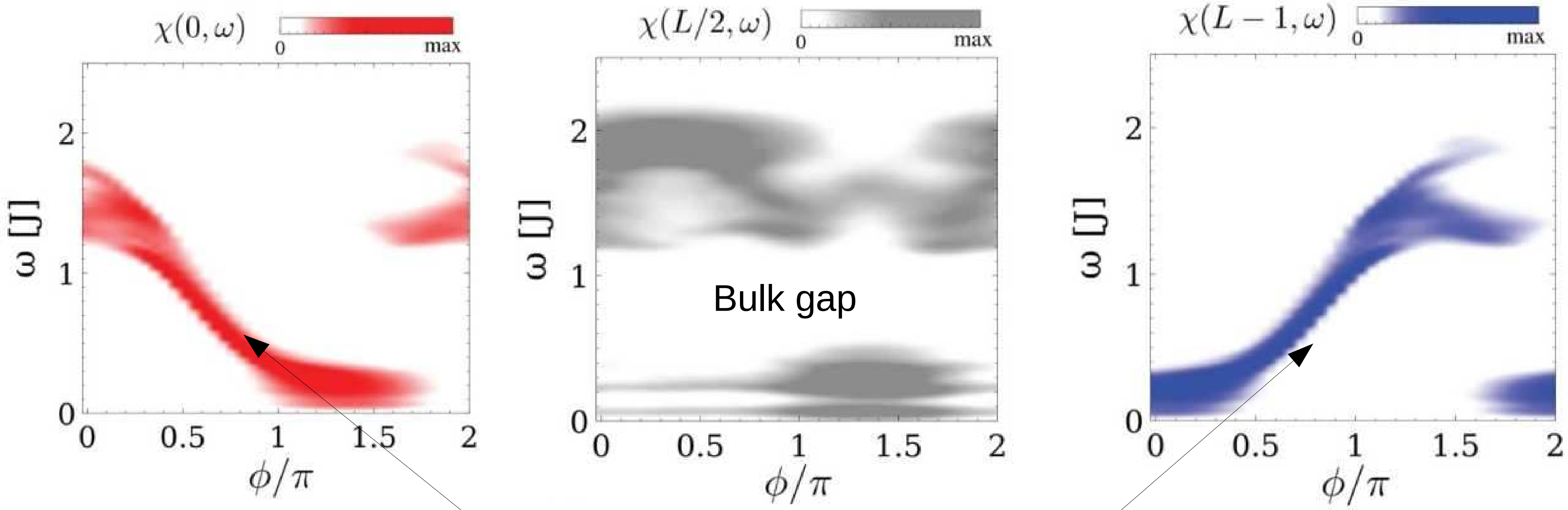




Quasiperiodic many-body interactions create topological spinon modes

Topological quasiperiodic spinons for S=1/2

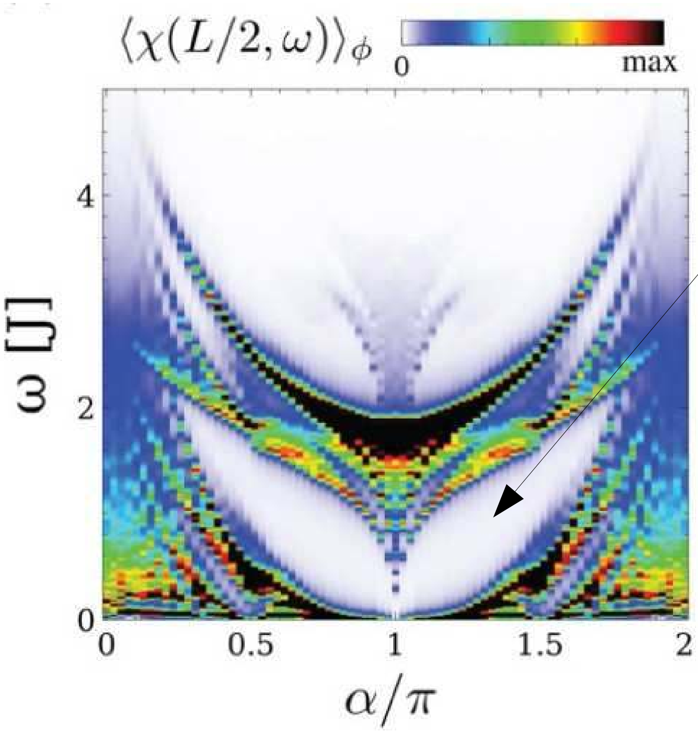
Left edge ***Bulk*** ***Right edge***



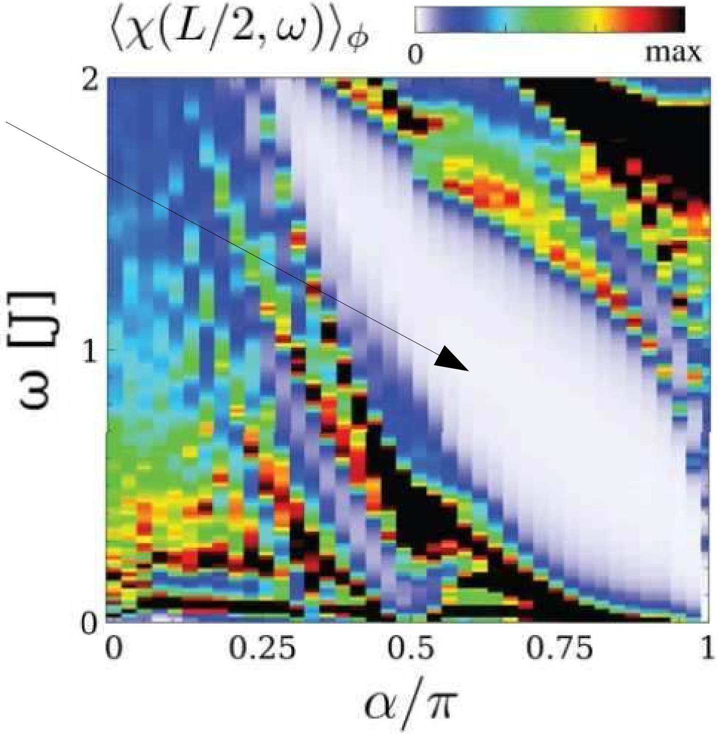
Topological spinon pumping modes

$$H = J\sum_{N}[1+\lambda\cos(\alpha N+\phi)]\vec{S}_N\cdot\vec{S}_{N+1}$$

Spinon Hofstadter spectra S=1/2



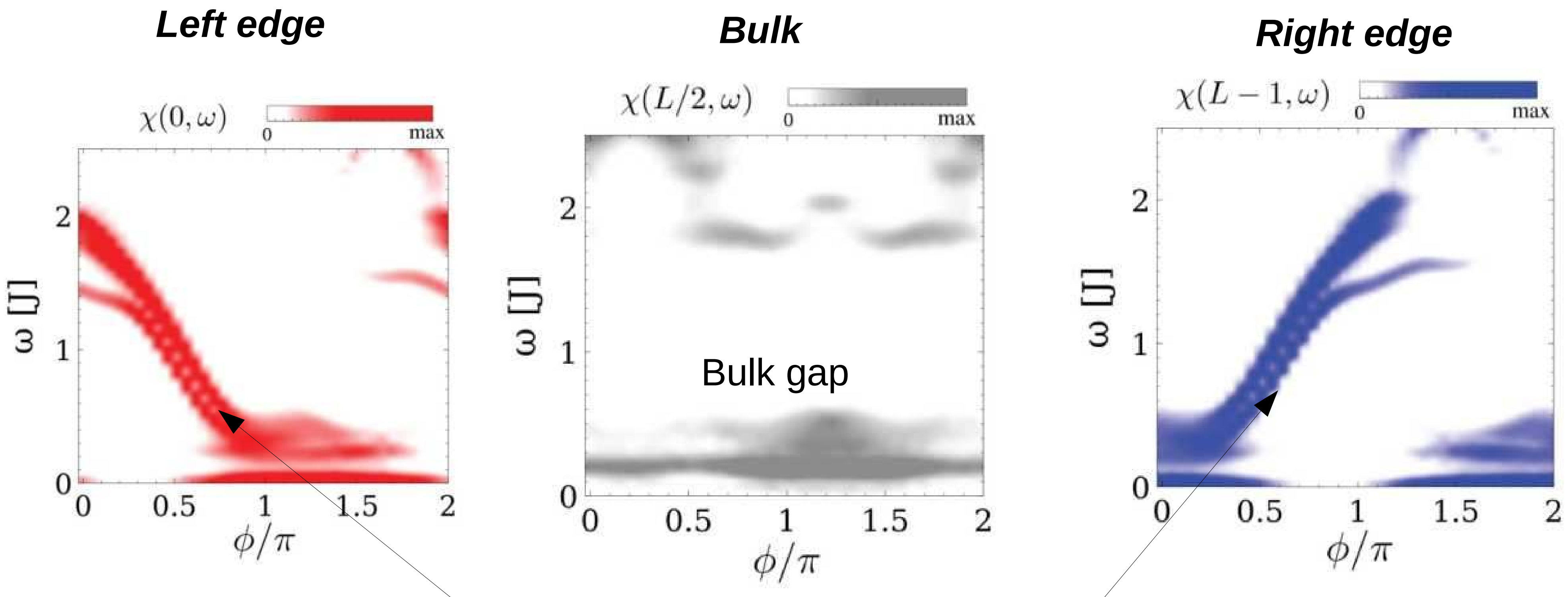
Topological gap



$$H = J\sum_N [1+\lambda\cos(\alpha N+\phi)]\vec{S}_N\cdot\vec{S}_{N+1}$$

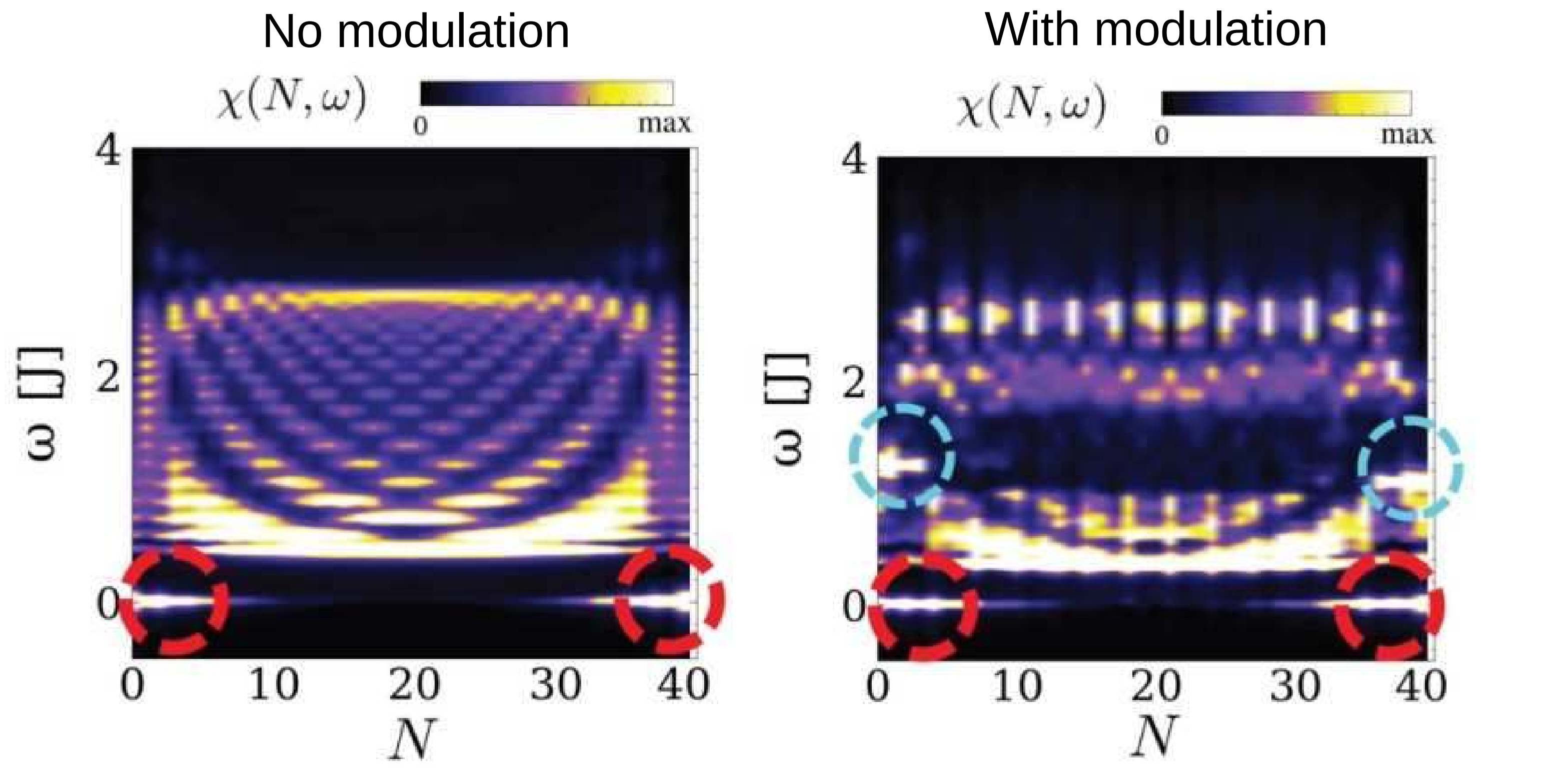
Topological gaps appear for arbitrary quasiperiodicity

Topological quasiperiodic spinons for S=1



$$H = J\sum_N [1+\lambda\cos(\alpha N+\phi)]\vec{S}_N\cdot\vec{S}_{N+1}$$

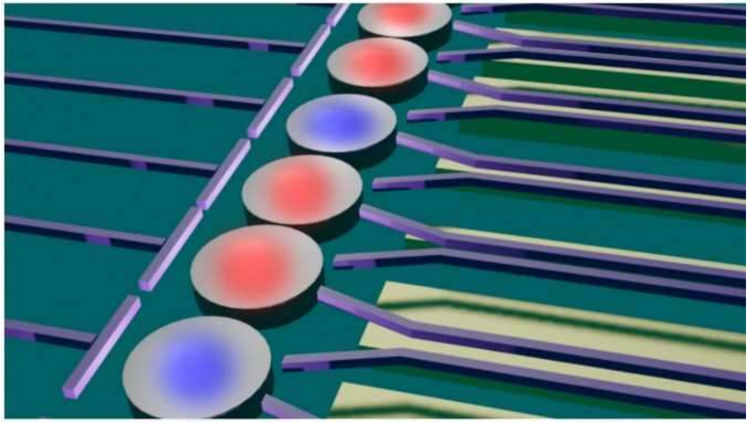
Topological quasiperiodic spinons for S=1

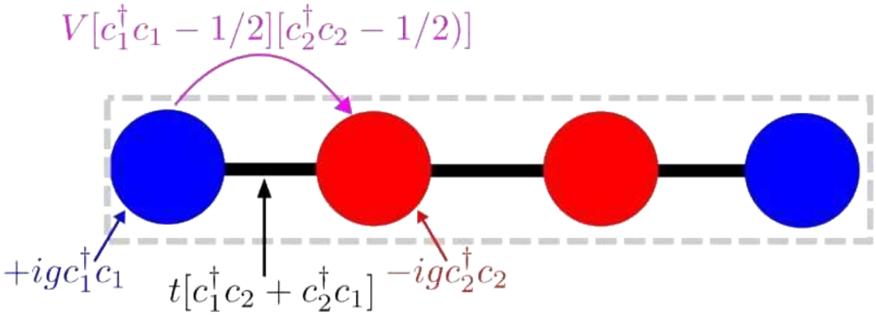


Quasiperiodicity creates additional topological modes away from E=0

Non-Hermitian topological many-body excitations

Topological excitations driven by modulated losses





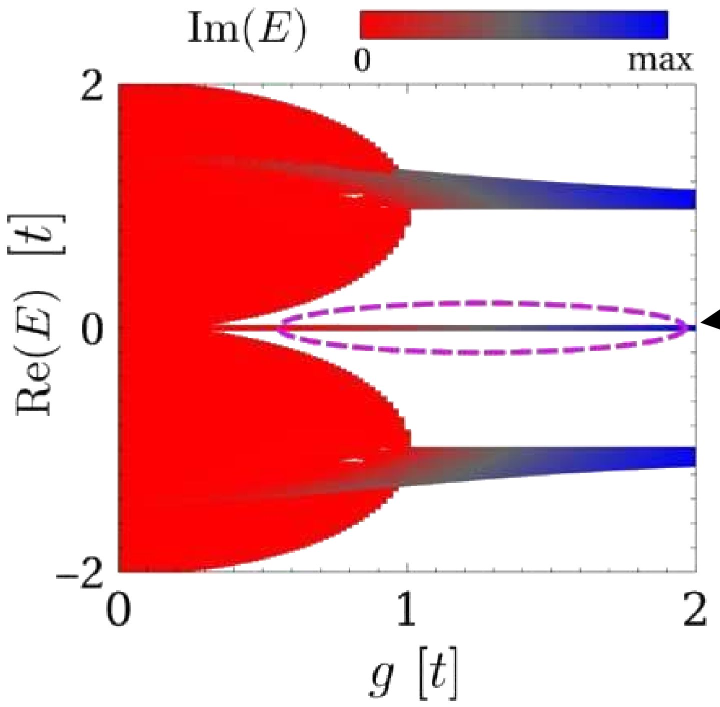
$$H_k = \begin{pmatrix} ig_1 & t & 0 & te^{-ik} \\ t & ig_2 & t & 0 \\ 0 & t & ig_3 & t \\ te^{ik} & 0 & t & ig_4 \end{pmatrix}$$

$$\Sigma_i(E) = \tilde{E}_i - ig_i,$$

Losses coming from a self-energy

Edge mode driven by losses

Non-interacting spectra



Edge state

Does this topological mode survive the presence of many-body interactions?

Looking for a non-Hermitian edge mode

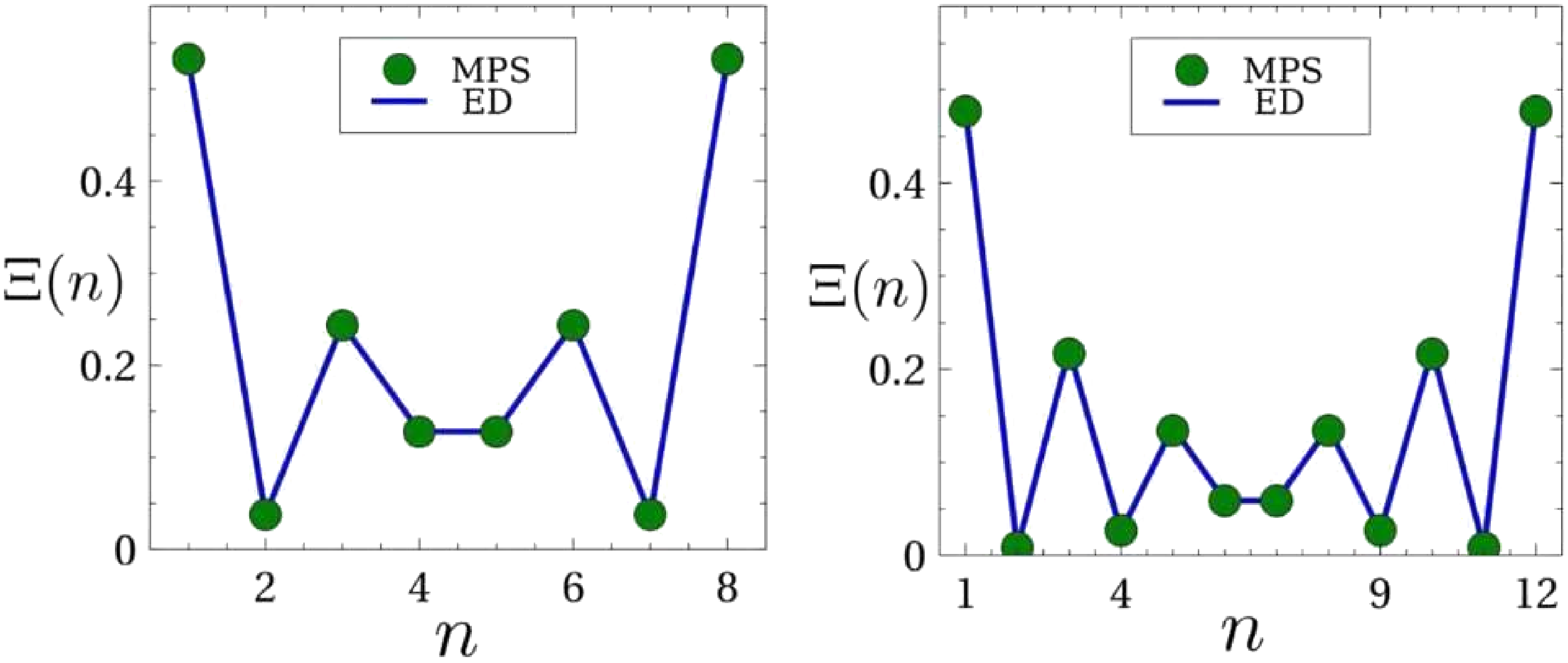
- As the Hamiltonian is non-Hermitian, DMRG cannot be used
- The ground state and excited is obtained using a non-Hermitian Krylov-Arnoldi iterative solver with matrix-product states
- The edge modes are imaged by the correlator

$$\Xi(n) = \sum_i |\langle \Psi_i | c_n | \Omega \rangle|^2.$$

Degenerate energy manifold

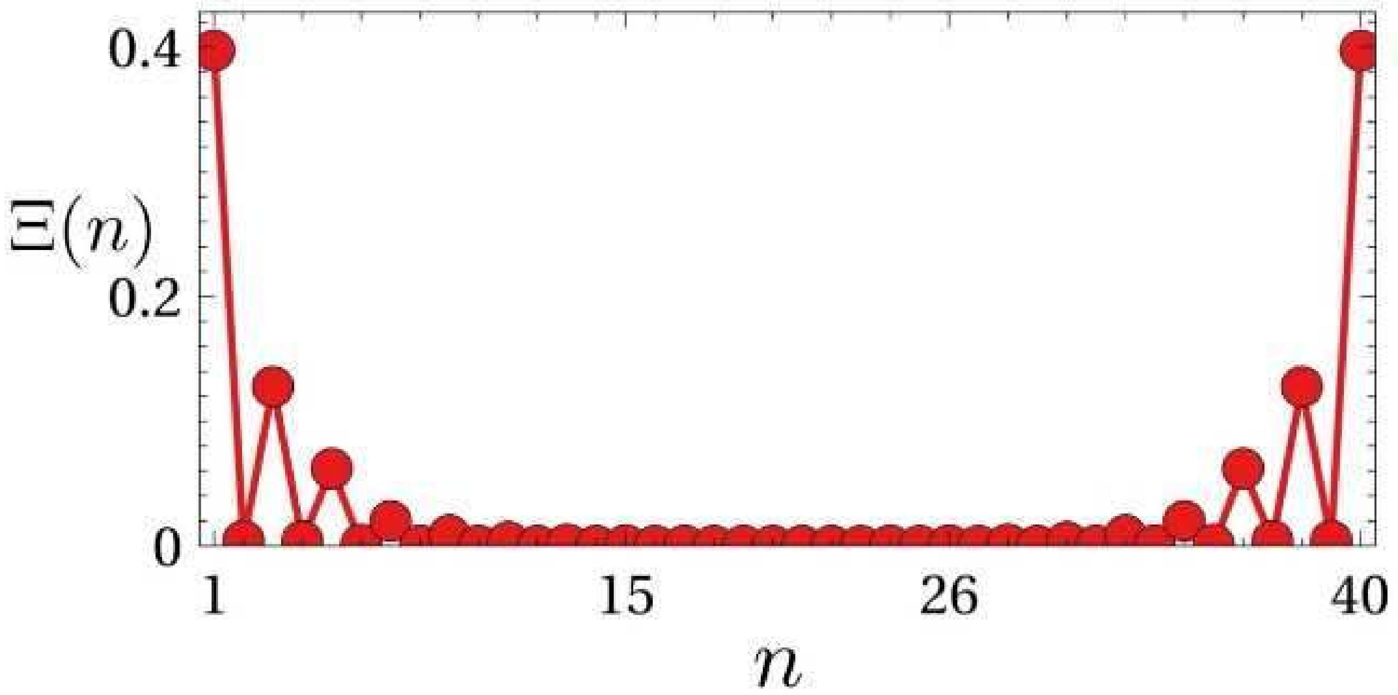
Ground state

Non-Hermitian edge modes



In short chains two overlapping edge modes appear in the correlator

Non-Hermitian edge modes



In long chains solved with MPS, the non-Hermitian mode becomes well localized at the edge

Dynamical correlator of many-body non-Hermitian model

In a non-Hermitian model, the dynamical correlator cannot be compute with a usual Kernel polynomial expansion

$$\mathcal{S}(\omega, l) = \langle \mathrm{GS_L}| S_l^- \delta^2(\omega + E_{\mathrm{GS}} - H) S_l^+ |\mathrm{GS_R}\rangle + \langle \mathrm{GS_L}| S_l^+ \delta^2(\omega + E_{\mathrm{GS}} - H) S_l^- |\mathrm{GS_R}\rangle,$$

We define a Hermitrized Hamiltonian

$$\mathcal{H} = \begin{pmatrix} & \omega - H \\ \omega^* - H^\dagger & \end{pmatrix}$$

And perform a KPM expansion of

$$f(\omega) = \langle \psi_\mathrm{L}|\delta^2(\omega - H)|\psi_\mathrm{R}\rangle$$

$$f(\omega) = \frac{1}{\pi}\partial_{\omega^*} G(E=0)$$

$$G(E) = \langle \mathrm{L}|(E - \mathcal{H})^{-1}|\mathrm{R}\rangle$$

Dynamical correlator of a topological non-Hermitian model

We take the following non-Hermitian model

Drives skin effect

$$\tilde{H} = \sum_{l=1}^{L-1} \Big(\frac{J+\gamma}{2} c_l^\dagger c_{l+1} + \frac{J-\gamma}{2} c_{l+1}^\dagger c_l$$

$$+ J_z (c_l^\dagger c_l - \frac{1}{2})(c_{l+1}^\dagger c_{l+1} - \frac{1}{2}) \Big) + \sum_{l=1}^{L} i h_l^z (c_l^\dagger c_l - \frac{1}{2}).$$

Drives topology

Full dynamical correlator

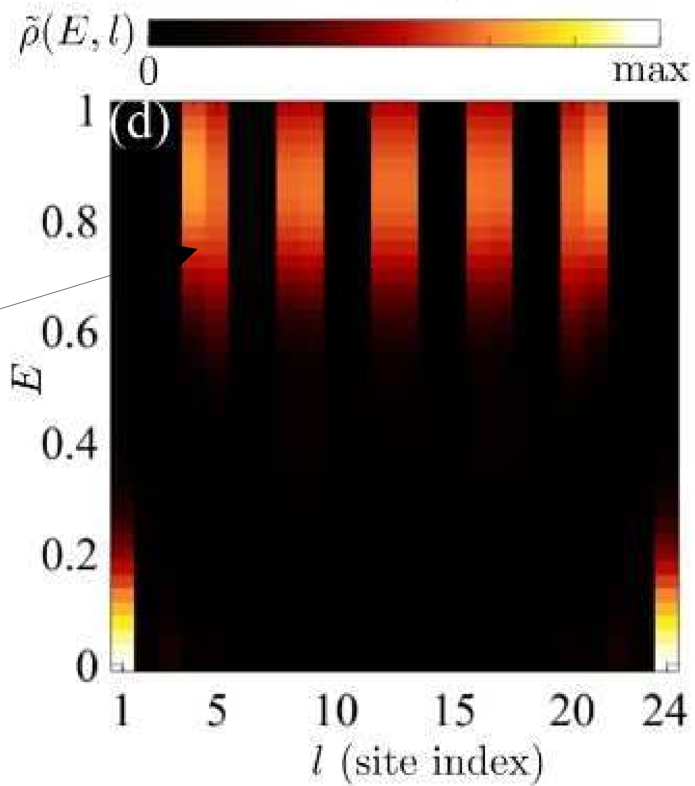
$$\mathcal{S}(\omega, l) = \langle \mathrm{GS_L} | S_l^- \delta^2(\omega + E_{\mathrm{GS}} - H) S_l^+ | \mathrm{GS_R} \rangle + \langle \mathrm{GS_L} | S_l^+ \delta^2(\omega + E_{\mathrm{GS}} - H) S_l^- | \mathrm{GS_R} \rangle,$$

Integrated in the imaginary axis

$$\tilde{\rho}(E \in \mathbb{R}, l) = \left| \int \mathcal{S}(E + iy, l) dy \right|$$

(equivalent to the Hermitian one)

Non-Hermitian topological modes without skin effect

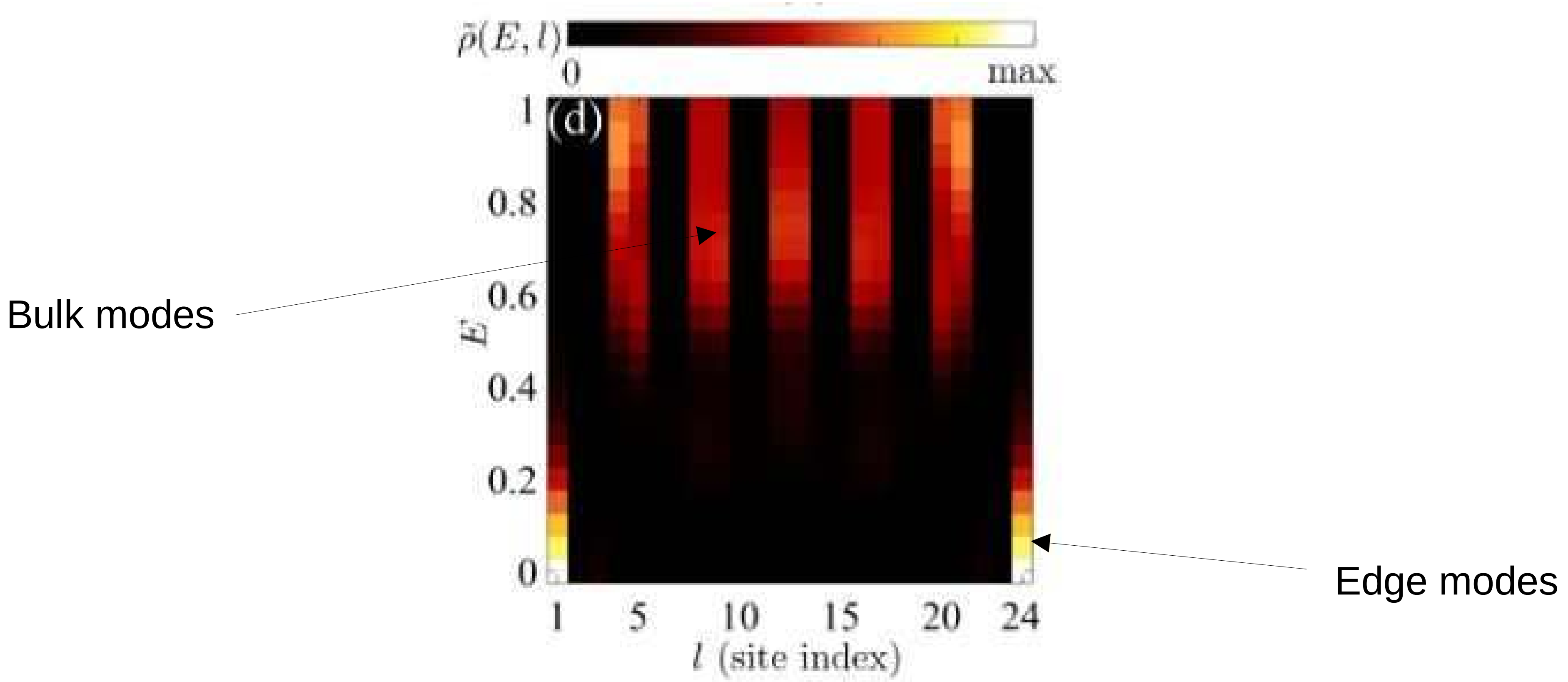


Bulk modes

Edge modes

The non-Hermitian dynamical correlator allows visualizing the topological modes

Non-Hermitian topological modes with skin effect



The non-Hermitian dynamical correlator allows visualizing the topological modes

Open-source software for tensor-network kernel polymonial algorithms

Open-source software for tensor-network kernel polymonial algorithms

dmrgpy

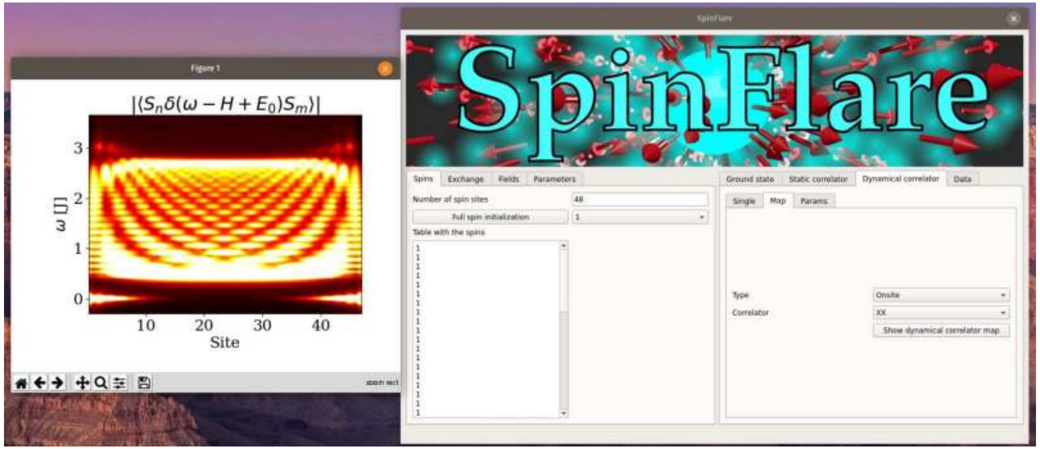
https://github.com/joselado/dmrgpy

```
from dmrgpy import spinchain
spins = ["S=1" for i in range(40)] # S=1 chain
sc = spinchain.Spin_Chain(spins) # create spin chain object
h = 0 # initialize Hamiltonian
for i in range(len(spins)-1):
  h = h + sc.Sx[i]*sc.Sx[i+1]
  h = h + sc.Sy[i]*sc.Sy[i+1]
  h = h + sc.Sz[i]*sc.Sz[i+1]
sc.set_hamiltonian(h)
sc.get_dynamical_correlator(name=(sc.Sz[0],sc.Sz[0]))
```

Generic Python library for tensor-network kernel polynomial algorithms for spins, fermions, parafermions

spinflare

https://github.com/joselado/spinflare

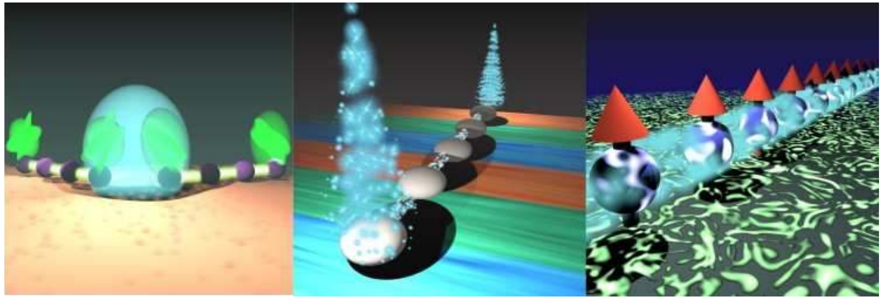


User friendly interface to compute excitations in quantum Heisenberg models

Based on ITensor

Take home

Tensor-network kernel polynomial algorithms allow computing dynamical excitations in quantum many-body systems



Thank you!

Phys. Rev. Research 1, 033009 (2019)
Phys. Rev. Research 3, 013265 (2021)
Phys. Rev. Research 3, 013095 (2021)
Phys. Rev. Research 4, L012006 (2022)
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