Quasiperiodic quantum many-body topology with the tensor-network kernel polynomial method

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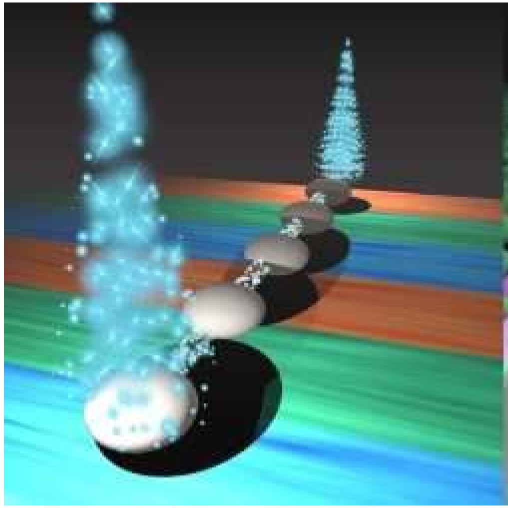
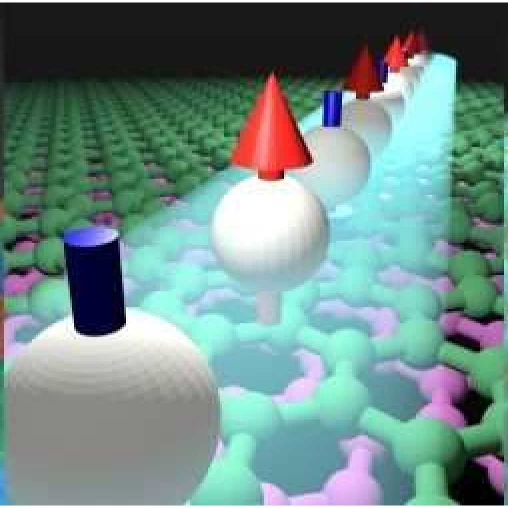
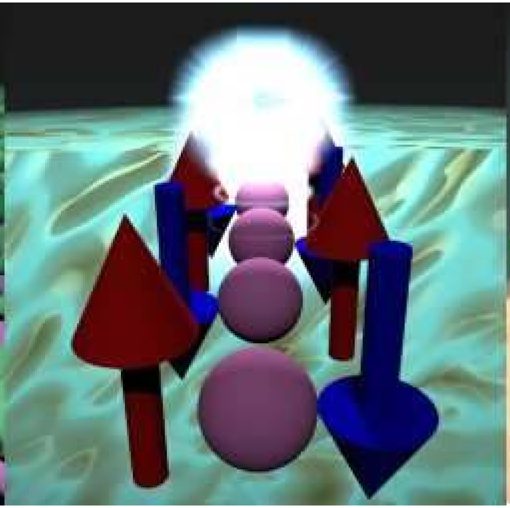


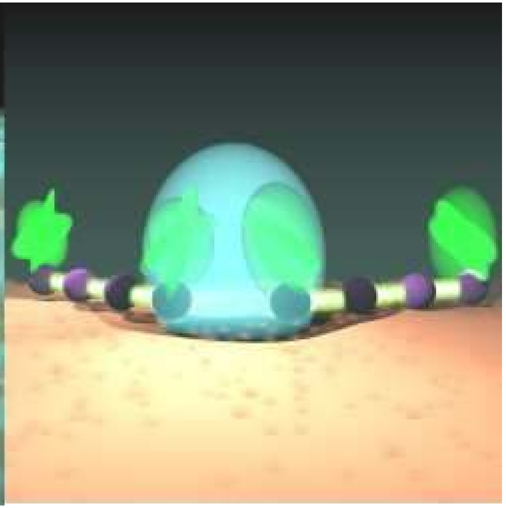
Phys. Rev. Research 3, 013265 (2021)



Phys. Rev. Research 1, 033009 (2019)



Phys. Rev. Research 2, 023347 (2020)

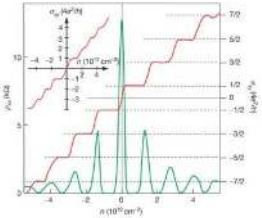


Phys. Rev. Research 3, 013095 (2021)

Real-space Simulations of Topological Matter and Disordered Materials, October 5th 2021

Topological matter

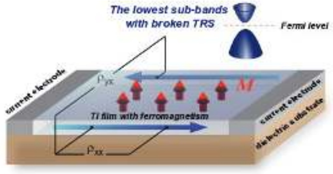
Quantum Hall effect



graphene

Nature 438, 197-200 (2005)

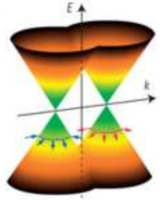
Quantum Anomalous Hall effect



Cr-doped $(Bi,Sb)_2Te_3$

Science 340.6129 (2013): 167-170

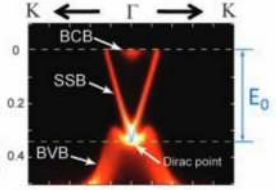
Weyl semimetal



TaAs

Nature Physics 11, 724–727 (2015)

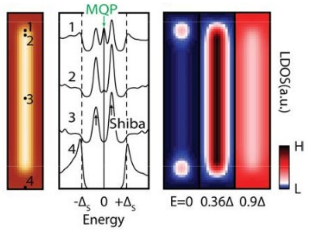
Quantum Spin Hall effect



Bi_2Se_3

Science 325.5937 (2009): 178-181

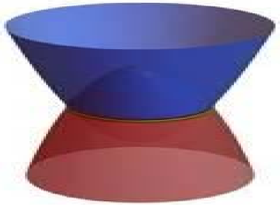
Topological superconductor



Fe@Pb

Science 346.6209 (2014): 602-607

Nodal line semimetals



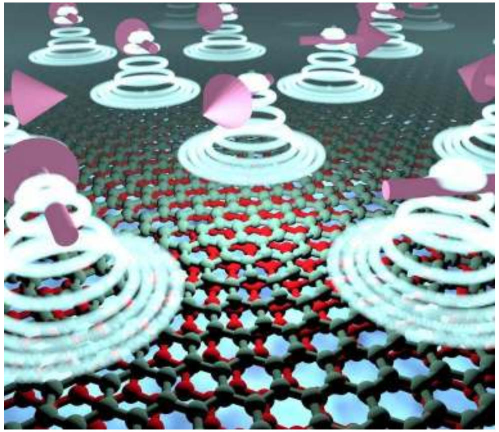
Mg_3Bi_2

Advanced Science 6.4 (2019): 1800897

All these states are described by effective single-particle Hamiltonians

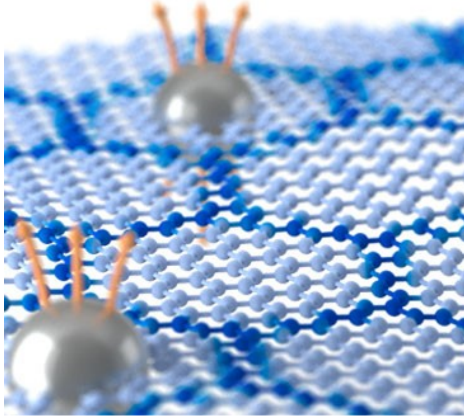
Many-body quantum matter

Quantum spin liquids



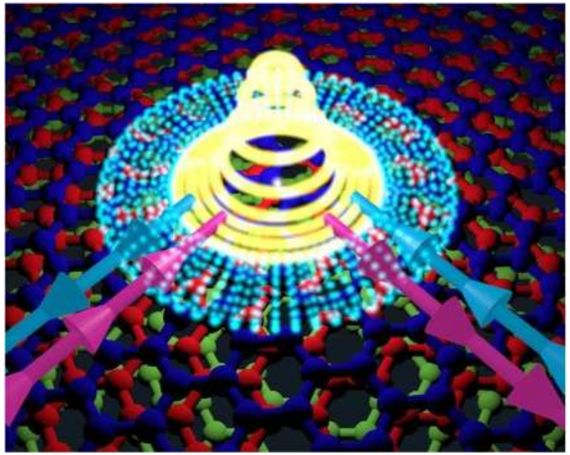
Reports on Progress in Physics 80.1 (2016): 016502.

Fractional Chern insulators



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

Parafermions



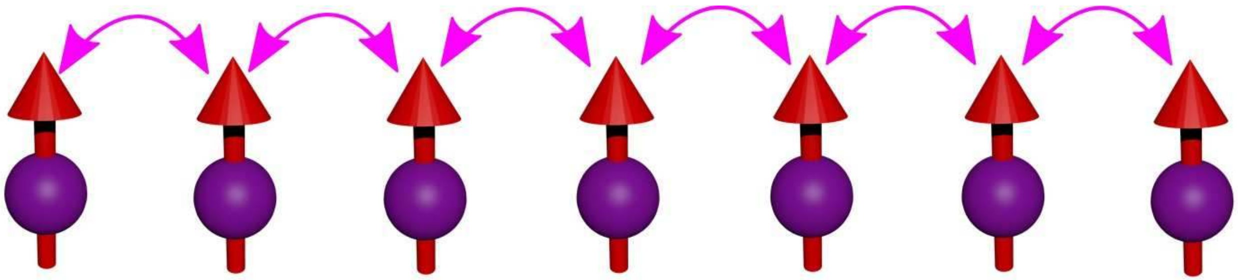
Annual Review of Condensed Matter Physics 7, 119-139 (2016)

Many-body quantum matter represents an exciting critically open challenge

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

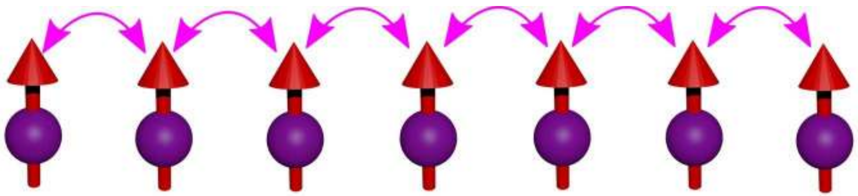
$$\mathcal{S}(N,\omega) = \langle GS | S_N^z \delta(\omega - \mathcal{H} + E_0) S_N^z | GS \rangle$$

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

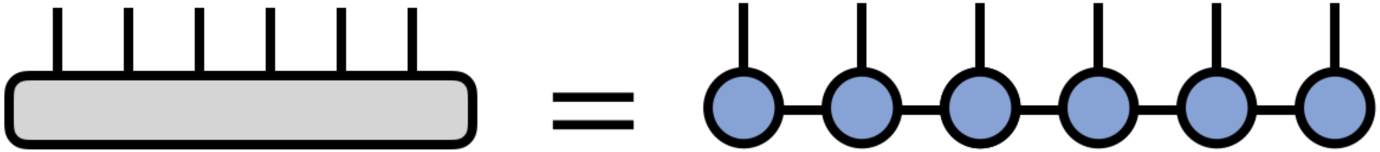
$$2^{30} \sim 10^9$$

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

State compression with tensor-networks

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

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



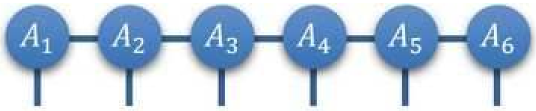
Matrix product state

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

Annals of Physics 326, 96 (2011)

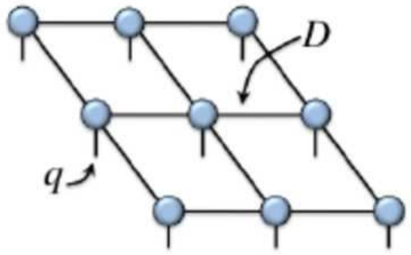
Many-body state compression

Matrix-product states



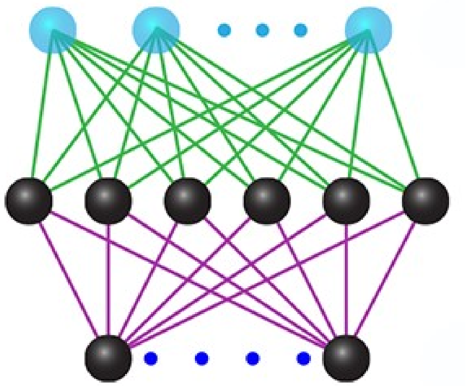
Phys. Rev. Lett. 69, 2863 (1992)

Projected entangled pair-states



Annals of Physics 326, 96 (2011)

Neural-network quantum states



Science 355.6325 (2017): 602-606.

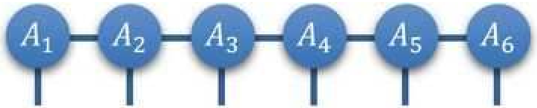
Compressed many-body states allow using kernel-polynomial methods for many-body systems

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

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

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

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

$$\mu_l = \langle \mathrm{GS} | S^z_N | w_l \rangle$$

$$|w_0\rangle = S^z_N |\mathrm{GS}\rangle,$$

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

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

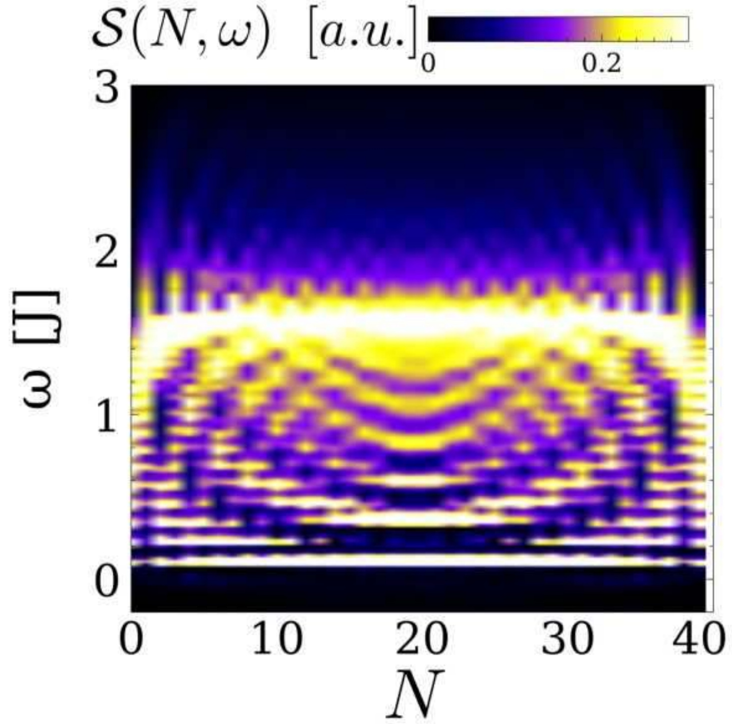
Rev. Mod. Phys. 78, 275 (2006)

Phys. Rev. Research 1, 033009 (2019)

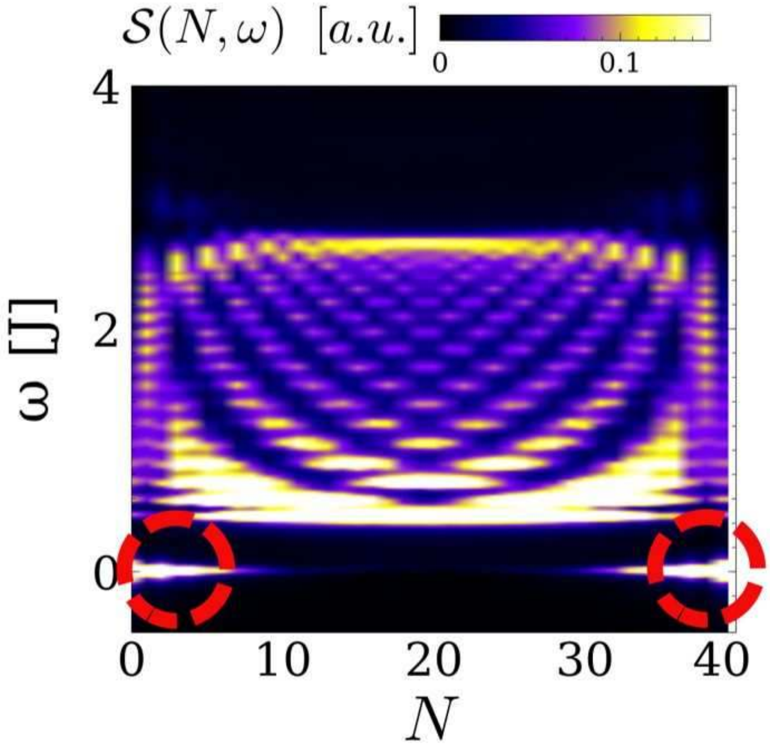
Open-source implementation in *https://github.com/joselado/dmrgpy*

Dynamical structure factor of a Heisenberg model

S=1/2 chain

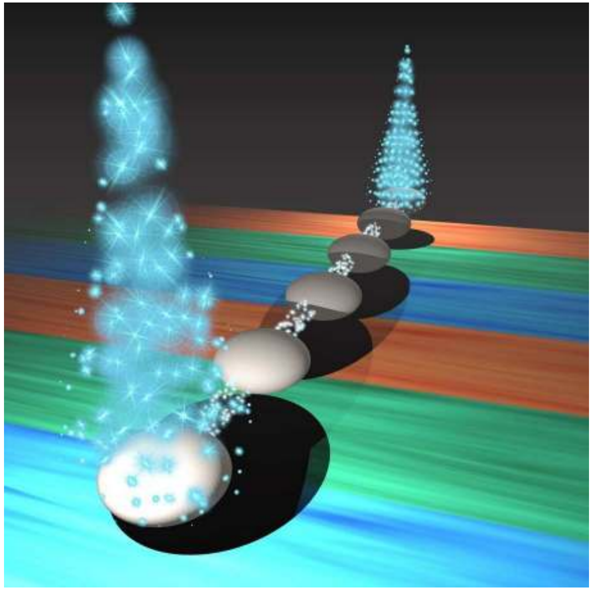


S=1 chain



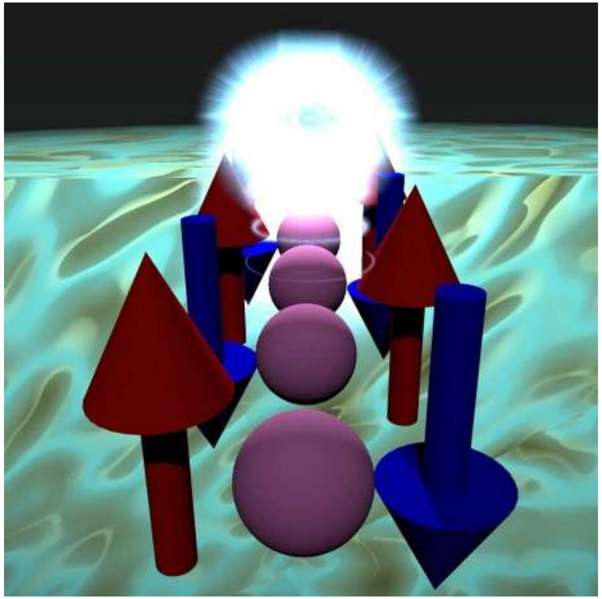
Today’s plan

Quasiperiodic many-body topology



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

Interface many-body topological modes



Phys. Rev. Research 2, 023347 (2020)
Phys. Rev. Research 3, 013095 (2021)

Behind the scenes

Malte Rösner

Phys. Rev. Research 3, 013265 (2021)

Quasiperiodic Coulomb topology

Oded Zilberberg

Phys. Rev. Research 1, 033009 (2019)

Quasiperiodic Heisenberg topology

Manfred Sigrist

Phys. Rev. Research 2, 023347 (2020)

Many-body quantum spin liquid-superconductor solitons

Vilja Kaskela

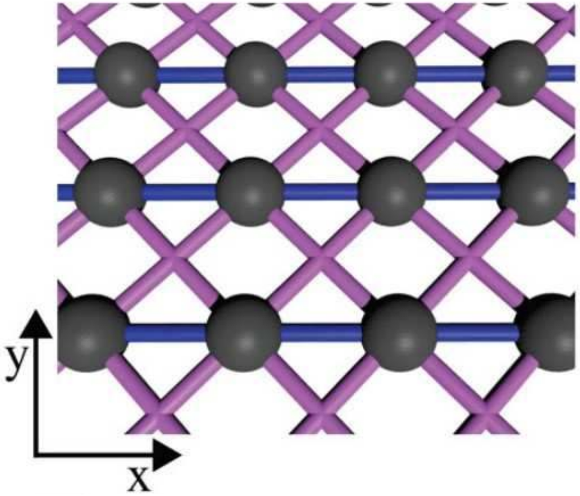
Phys. Rev. Research 3, 013095 (2021)

Many-body topological parafermion junctions

Coulomb modulated topology

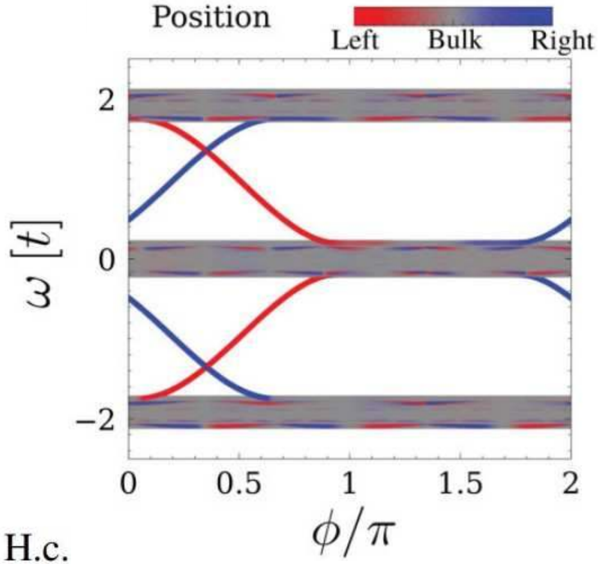
Quasiperiodic topology

Quantum Hall in a
two-dimensional lattice



$\sim$

Spectrum of the associated
quasiperiodic Hamiltonian



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

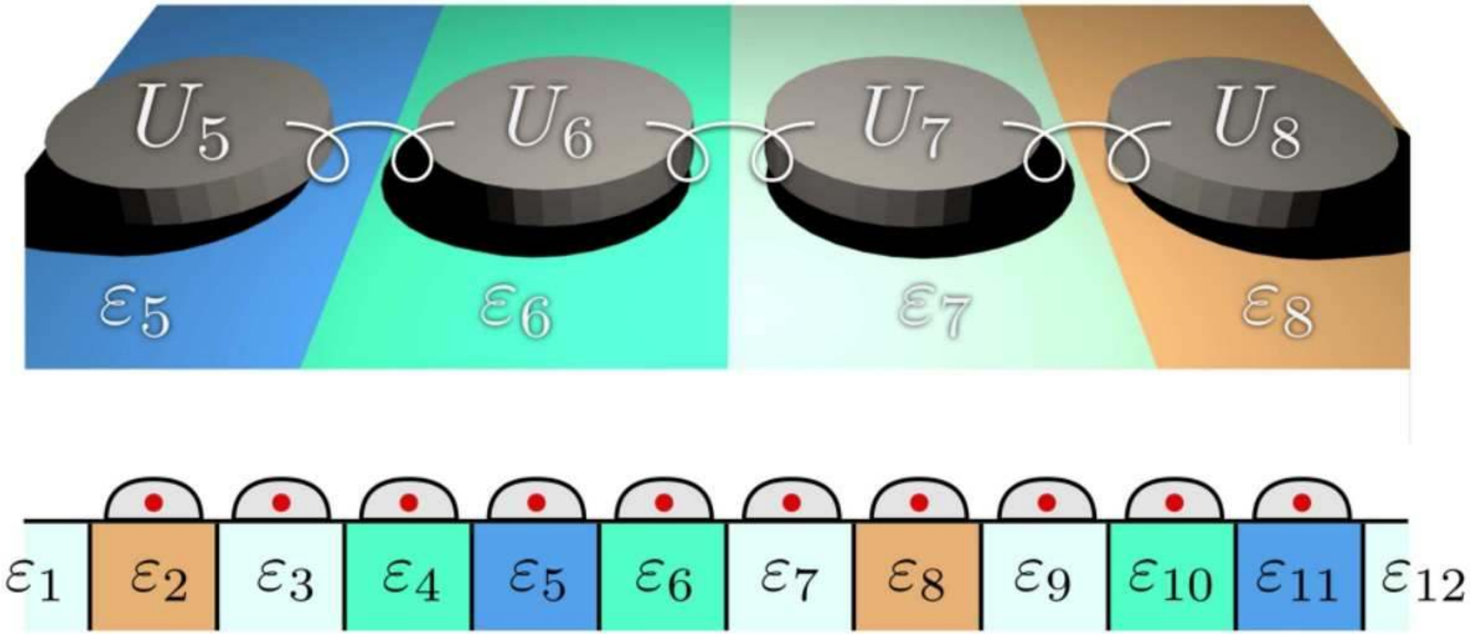
1D quasiperiodic models can be mapped to 2D quantum Hall states

This mapping is only valid in the non-interacting limit

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

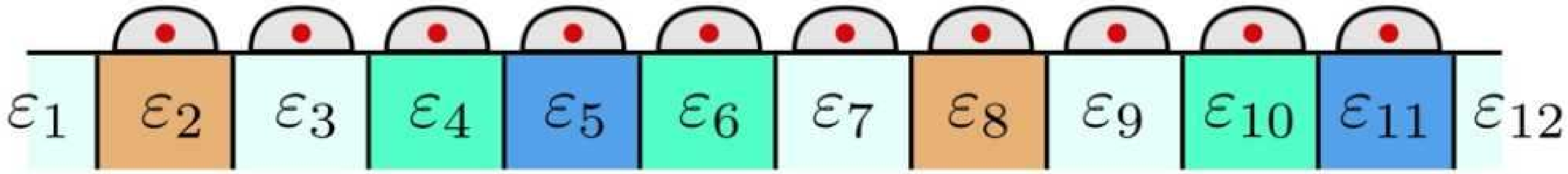
Many-body quasiperiodic interactions

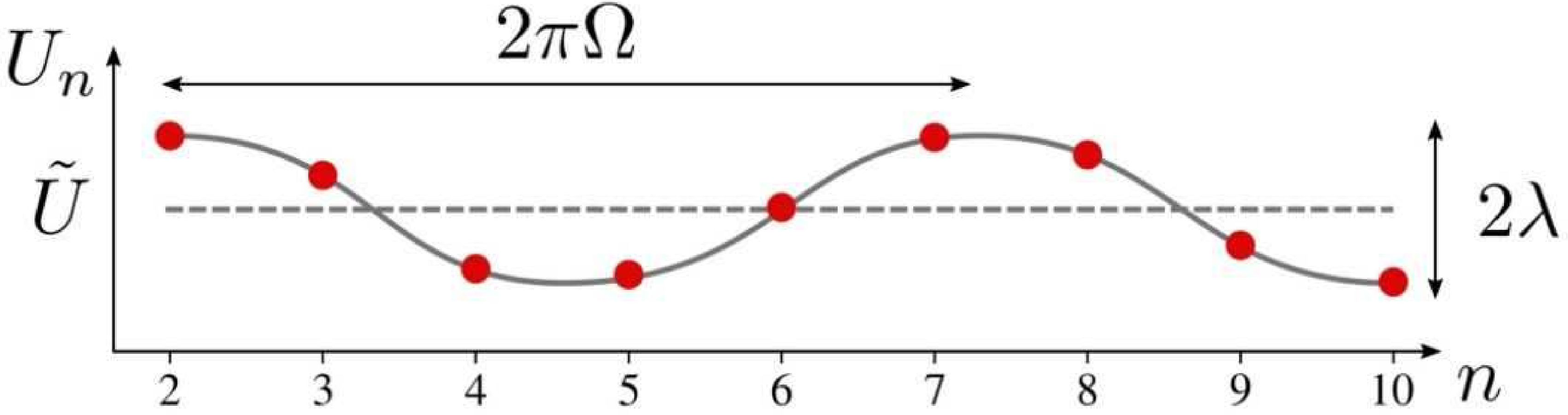
Substrate engineering allow creating spatially dependent interactions



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

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

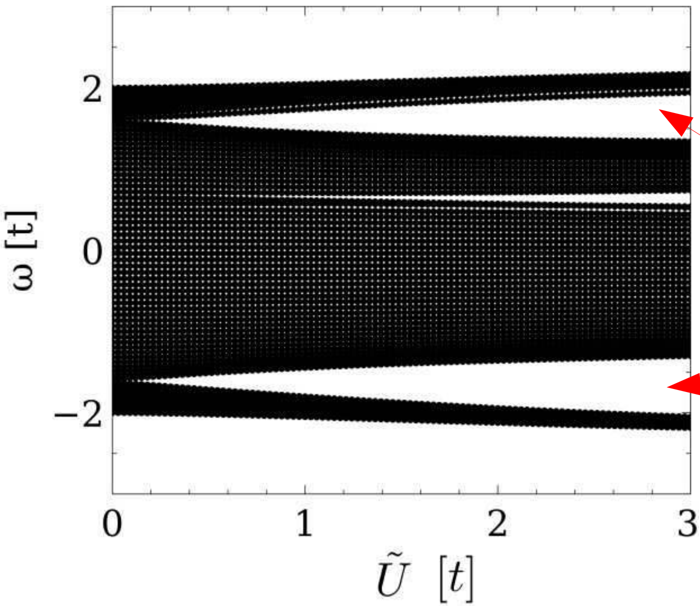
$$H = \sum_{n,s} t\, c^\dagger_{n,s} c_{n+1,s} + \sum_n U_n c^\dagger_{n,\uparrow} c_{n,\uparrow} c^\dagger_{n,\downarrow} c_{n,\downarrow} + h.c.$$

Modulated interactions

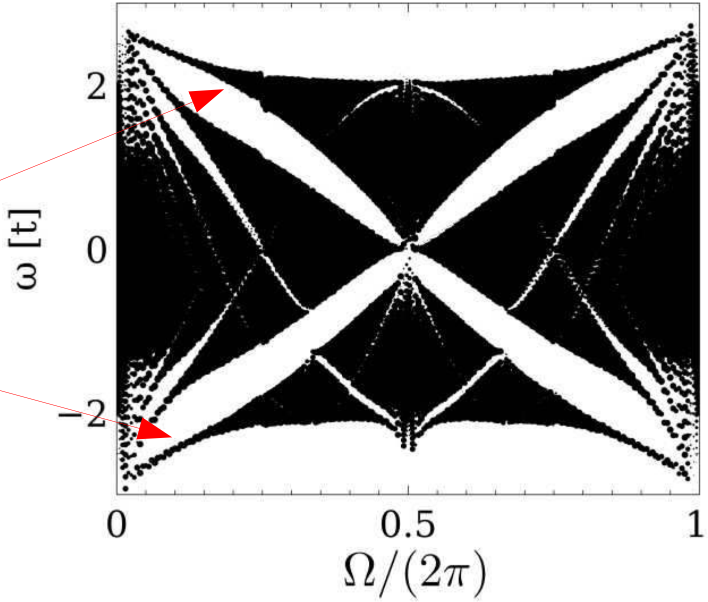
$$U_n = \tilde{U}[1 + \lambda \cos(\Omega n + \phi)]$$

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

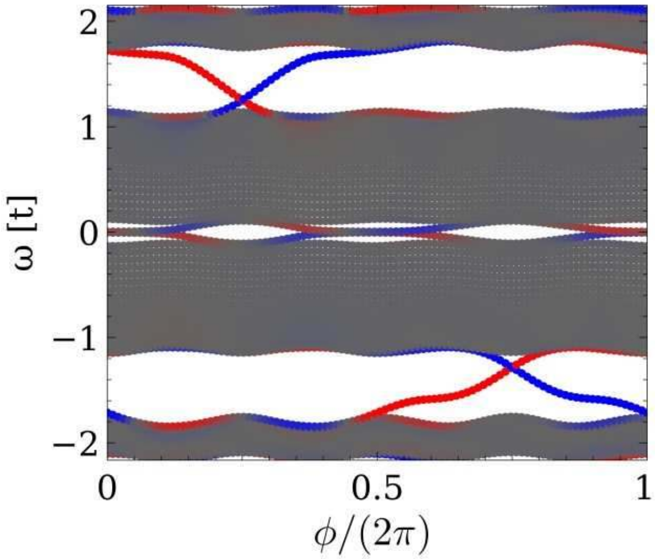


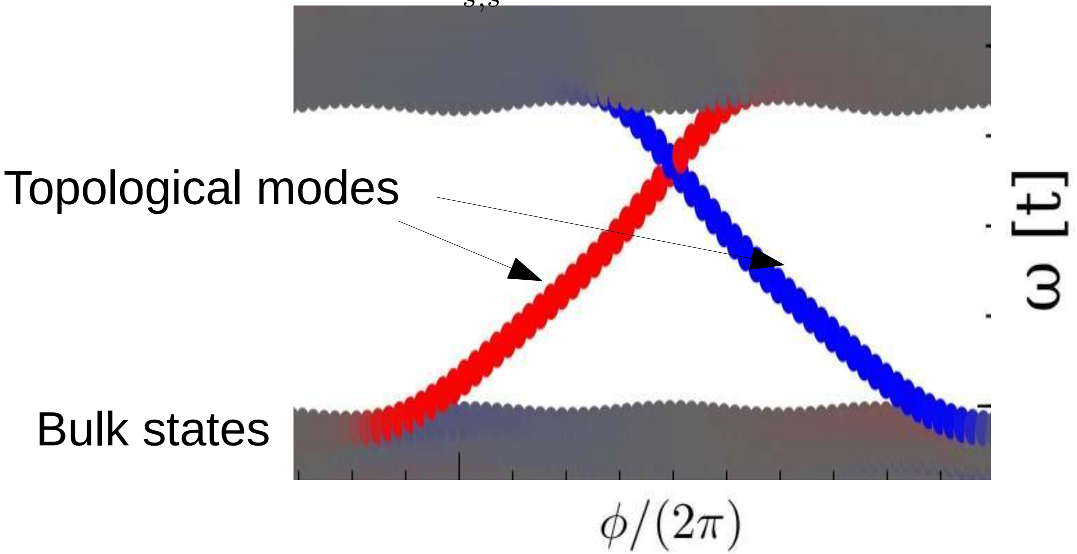
Warm-up: single particle Coulomb-engineered topology

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

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

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

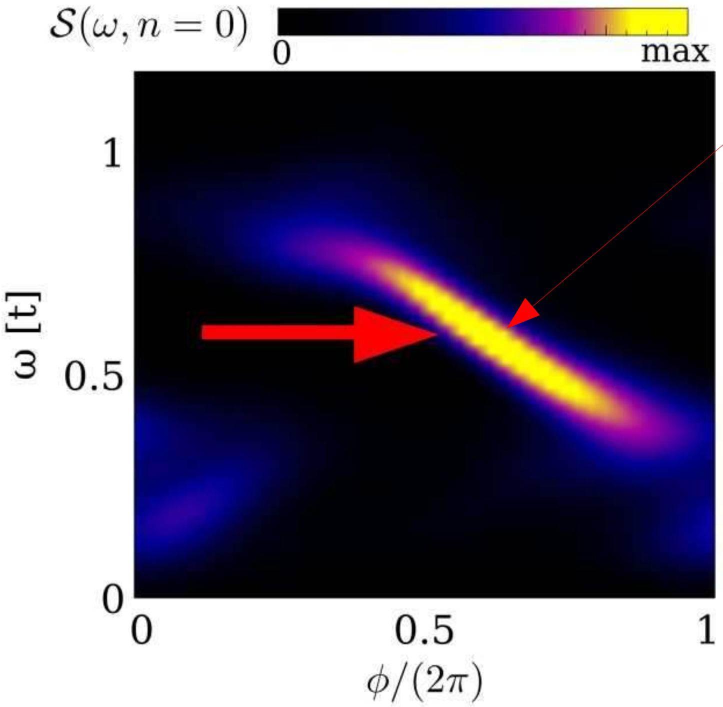
https://itensor.org/

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

https://github.com/joselado/dmrgpy

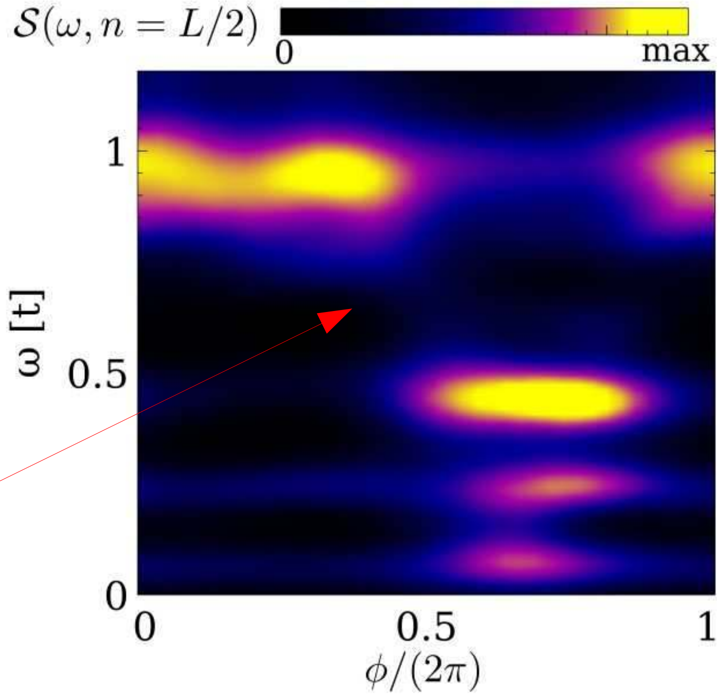
Many-body topological modes

Edge spectral function



Topological
edge mode

Bulk spectral function



Topological
bulk gap

Topological modes protected by a many-body quasiperiodic Chern invariant

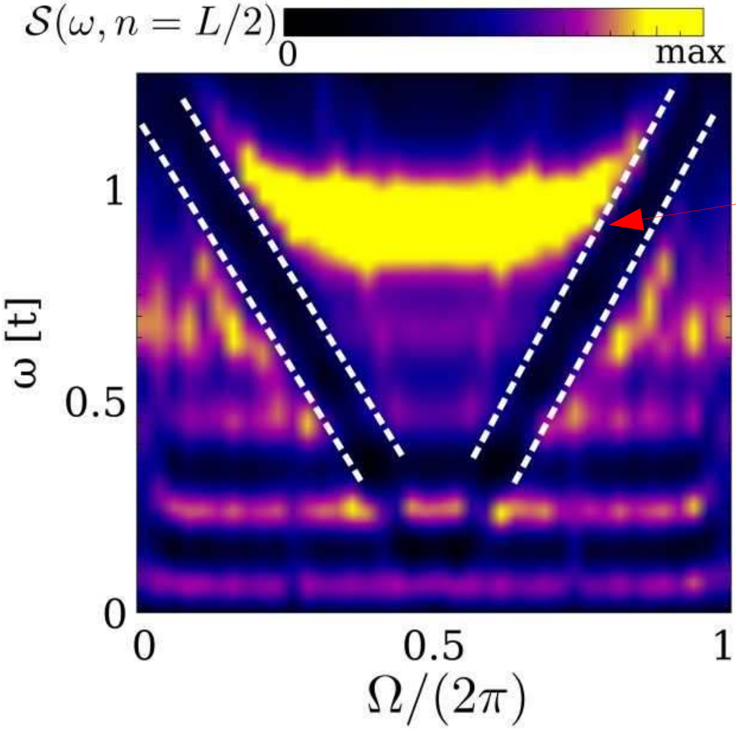
Phys. Rev. Research 1, 033009 (2020)

arXiv:2009.03752

arXiv:2010.06171

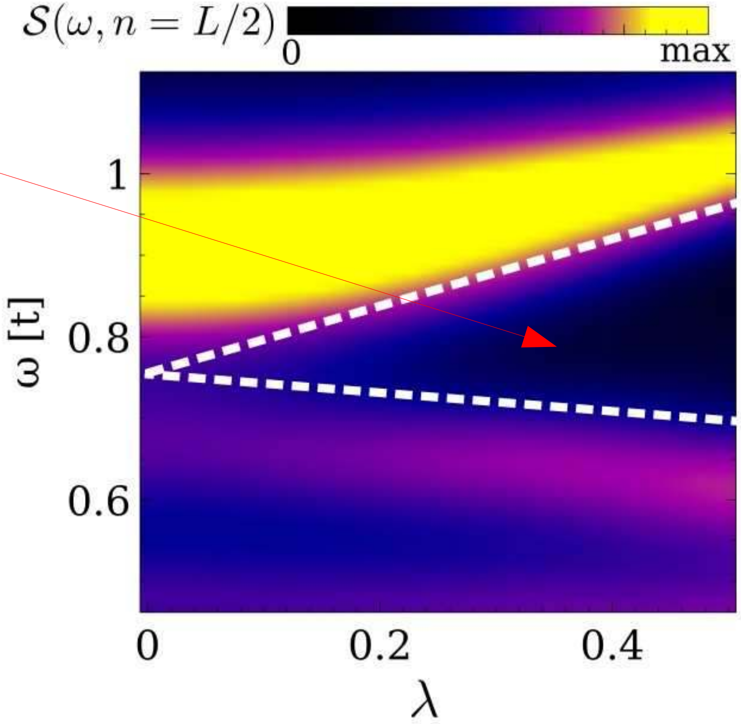
Many-body topological gaps

Bulk spectral function



Topological
bulk gap

Bulk spectral function



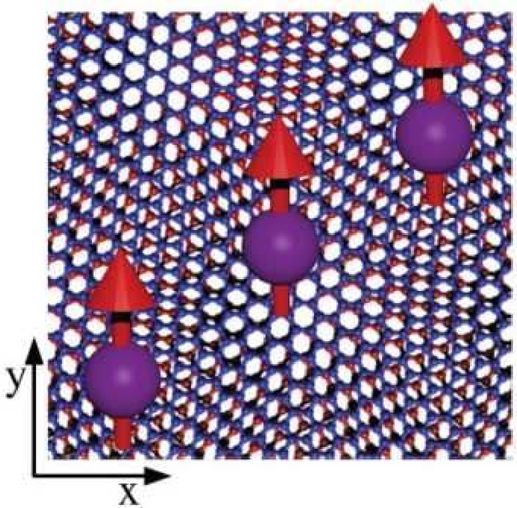
Topological gaps appear for generic modulation frequencies and strengths

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

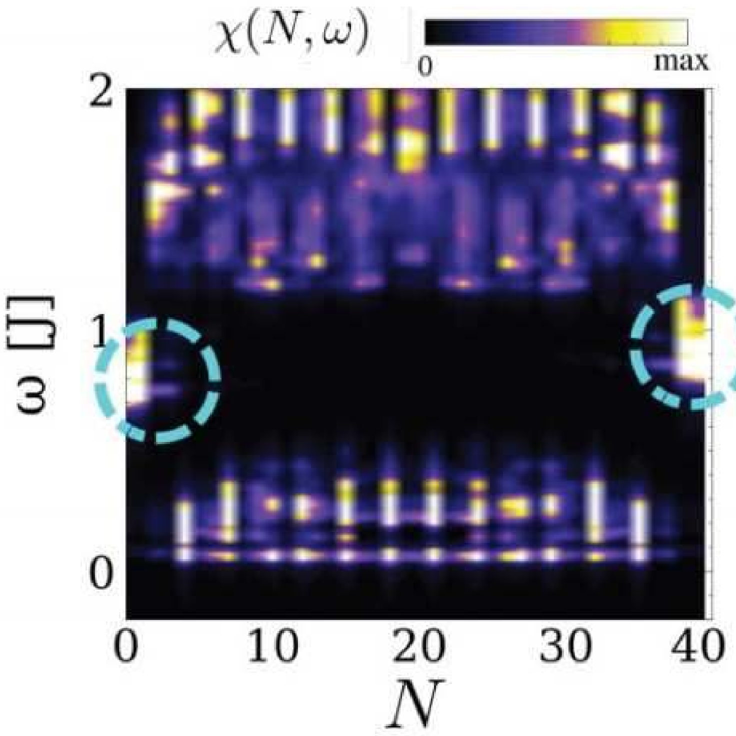


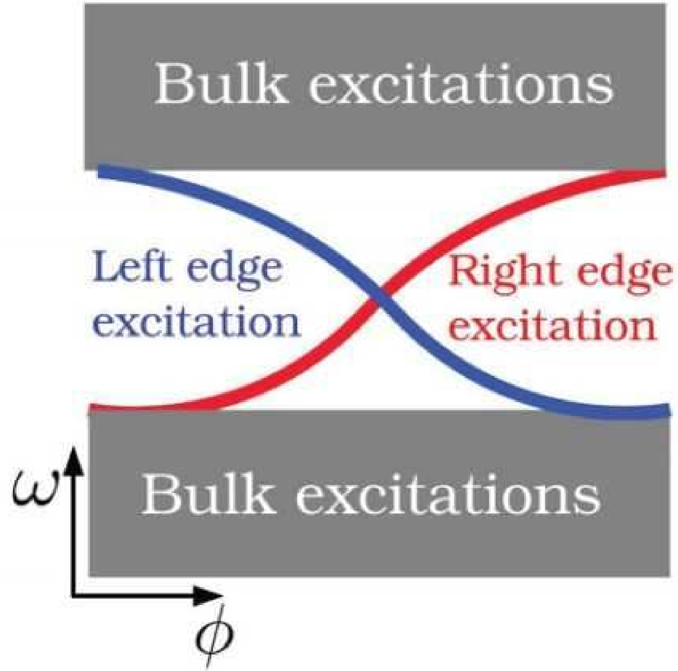
We will consider the generalized quasiperiodic Heisenberg model

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

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

Topological quasiperiodic spinon for S=1/2

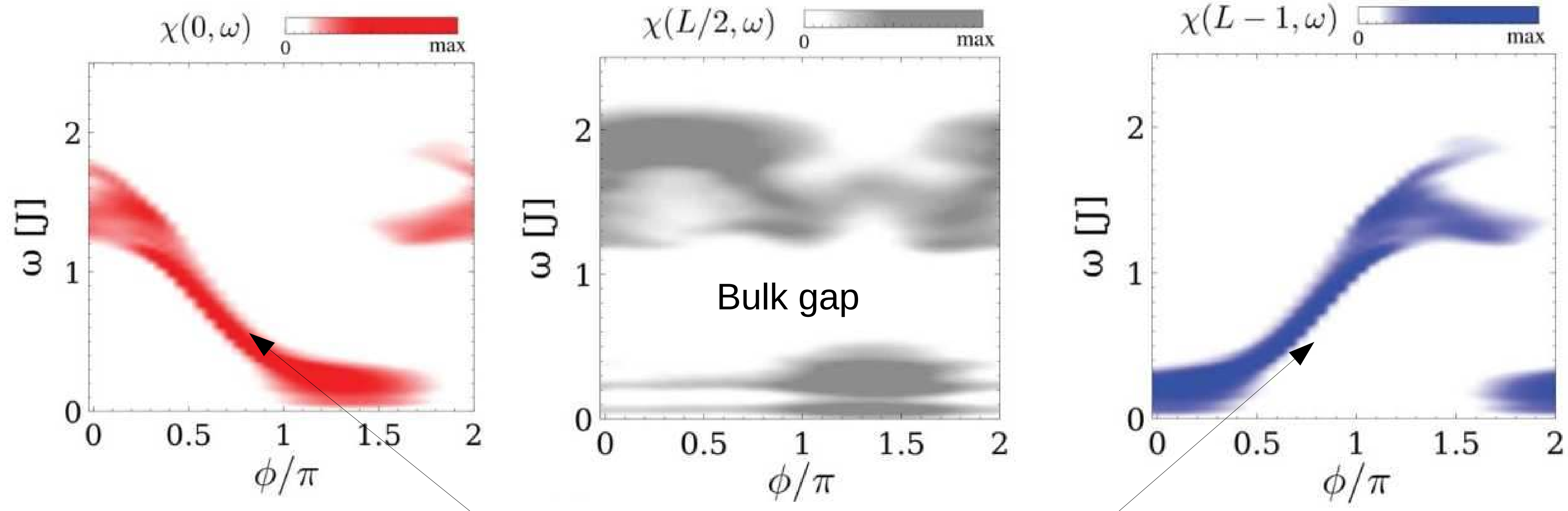




Quasiperiodic many-body interactions create topological spinon modes

Topological quasiperiodic spinons for S=1/2

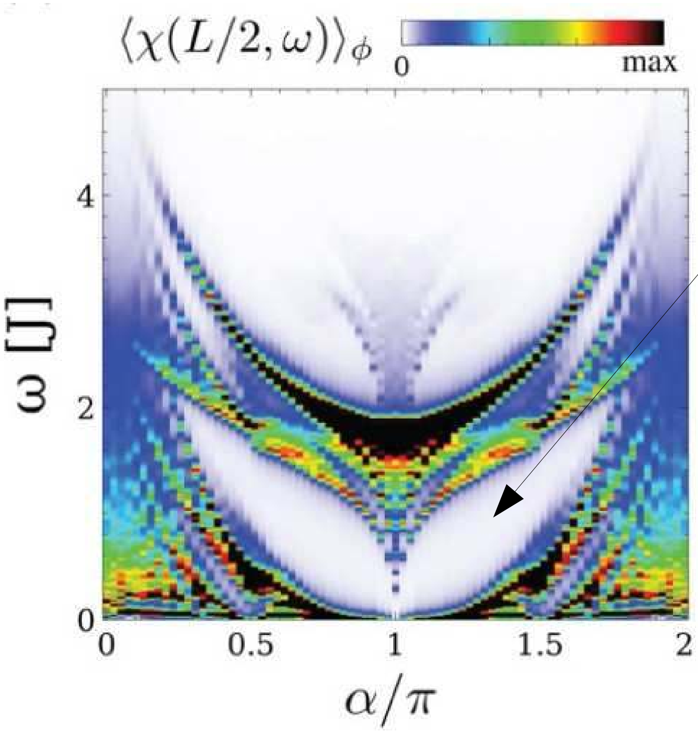
Left edge ***Bulk*** ***Right edge***



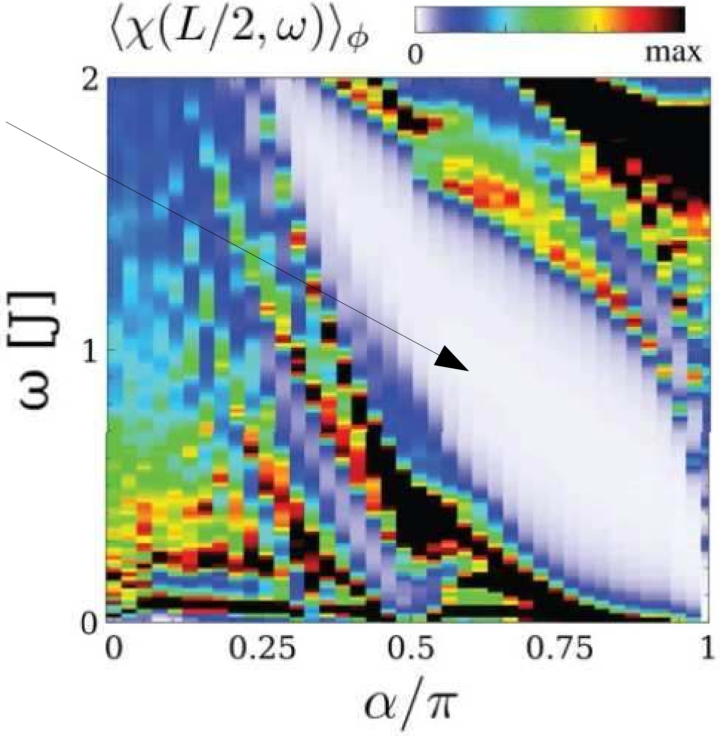
$$H = J\sum_N [1+\lambda\cos(\alpha N+\phi)]\vec{S}_N\cdot\vec{S}_{N+1}$$

Topological spinon pumping modes

Spinon Hofstadter spectra S=1/2



Topological gap

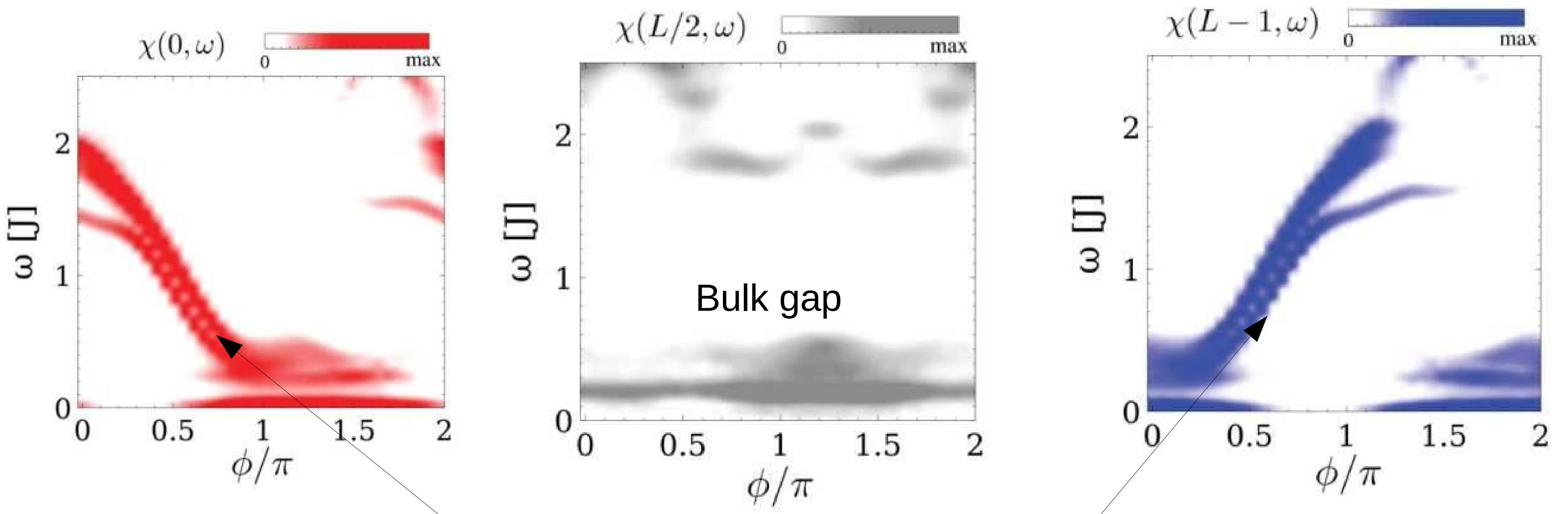


$$H = J \sum_N [1 + \lambda \cos(\alpha N + \phi)] \vec{S}_N \cdot \vec{S}_{N+1}$$

Topological gaps appear for arbitrary quasiperiodicity

Topological quasiperiodic spinons for S=1

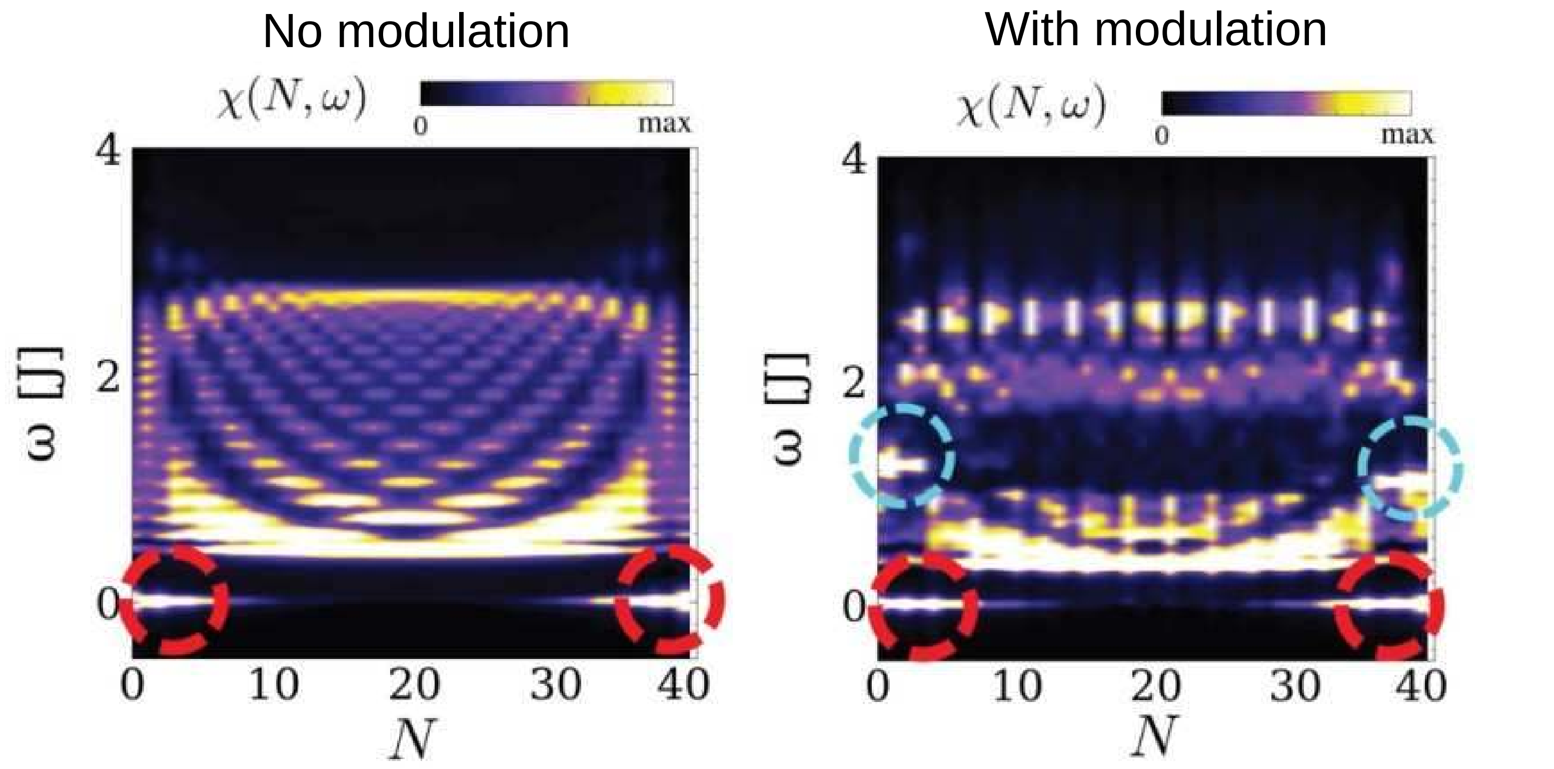
Left edge ***Bulk*** ***Right edge***



Topological spinon pumping modes

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

Topological quasiperiodic spinons for S=1



Quasiperiodicity creates additional topological modes away from E=0

Many-body excitations in quantum antiferromagnet-superconductor junctions

Quantum many-body antiferromagnets

Stagger antiferromagnet (mean-field solution)

$$\mathcal{H} = \mathcal{H}_{\mathrm{kin}} + \mathcal{H}_{\mathrm{AF}} \qquad |GS\rangle = |\uparrow\downarrow\rangle$$

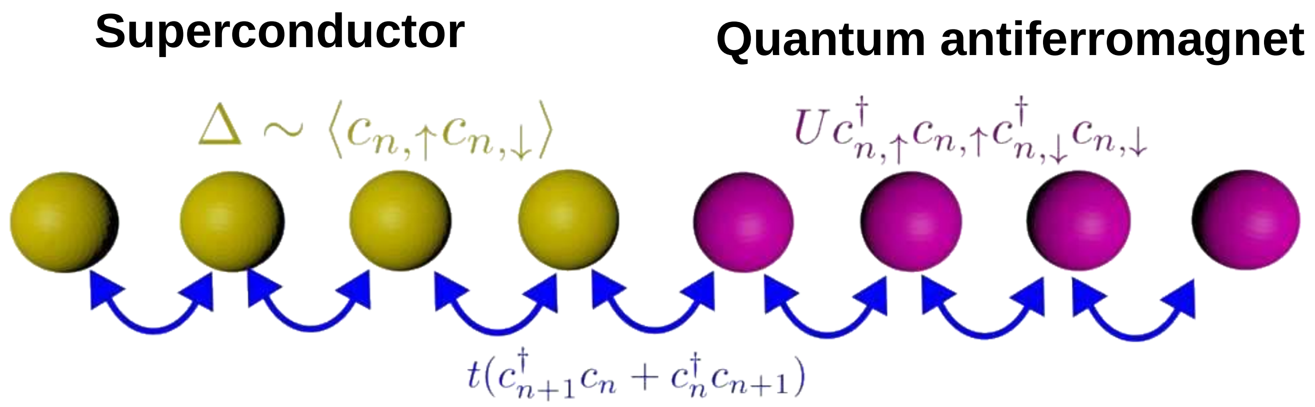
Quantum antiferromagnet (many-body solution)

$$\mathcal{H} = \mathcal{H}_{\mathrm{kin}} + \mathcal{H}_{\mathrm{U}} \qquad |GS\rangle = |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$$

Hubbard interaction $\mathcal{H}_{\mathrm{U}} = \sum_n U c^\dagger_{n,\uparrow} c_{n,\uparrow} c^\dagger_{n,\downarrow} c_{n,\downarrow}$

What happens at interfaces between a quantum many-body 1D antiferromagnet and a superconductor?

Superconductor-quantum antiferromagnet junction

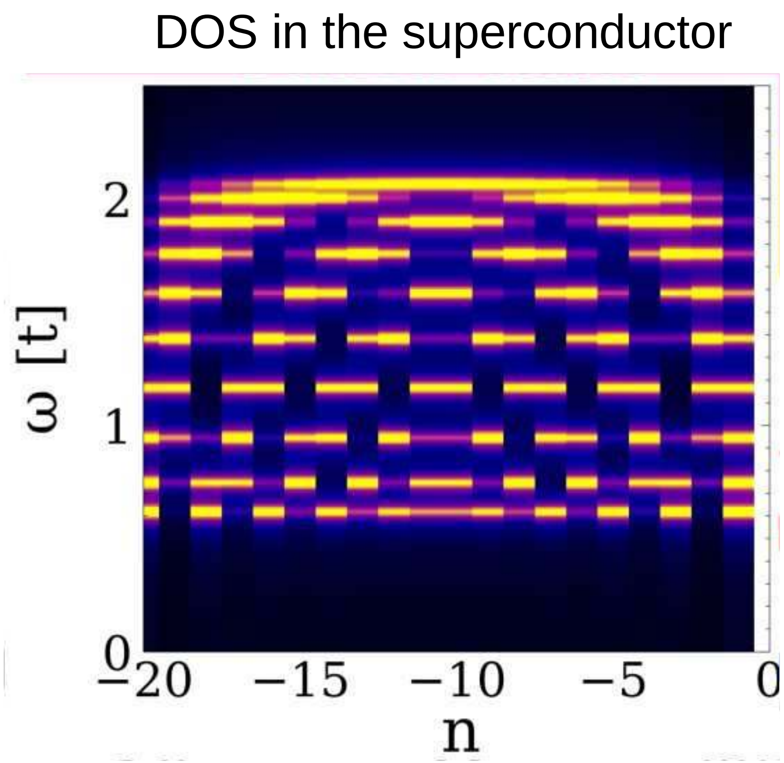


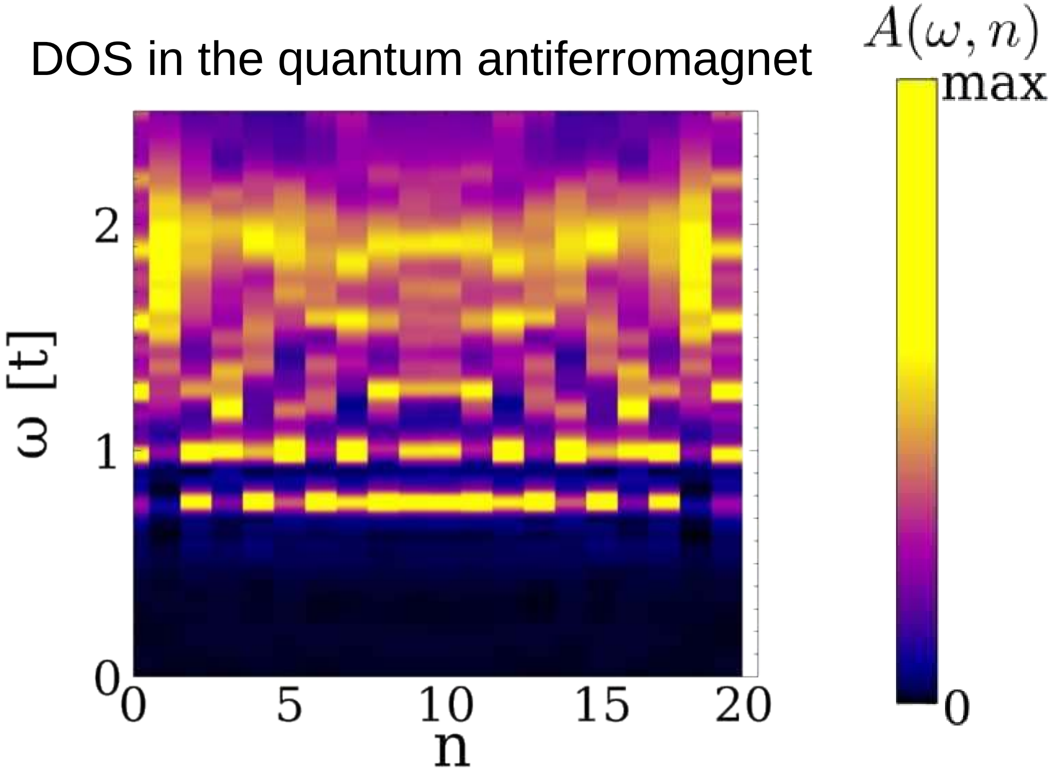
$$\mathcal{H} = \mathcal{H}_{\mathrm{kin}} + \mathcal{H}_{\mathrm{SC}} + \mathcal{H}_{\mathrm{int}}$$

We will solve the interacting model exactly using the tensor network formalism

<u>The ground state does not break time-reversal symmetry</u>

Many-body spectral function

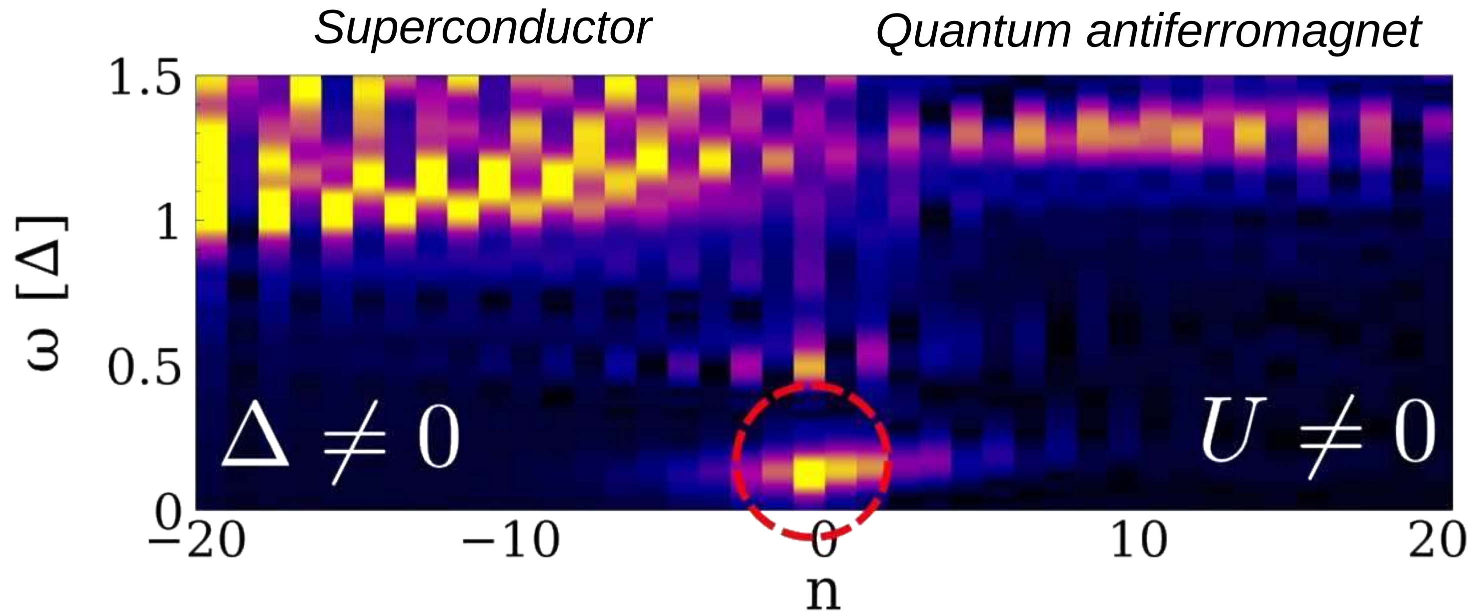




Both systems show an electronic gap when decoupled

In-gap modes at the SC-quantum AF interface

Superconductor-quantum antiferromagnet junction

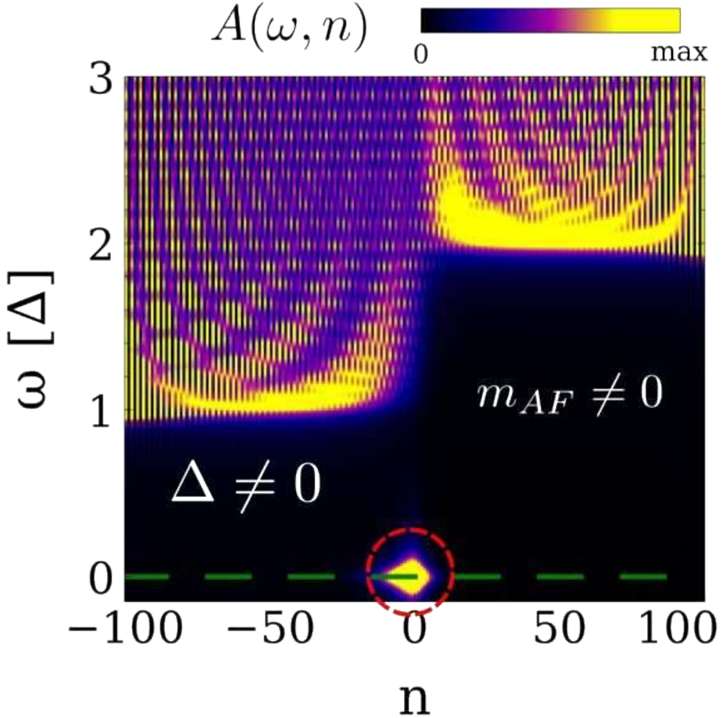


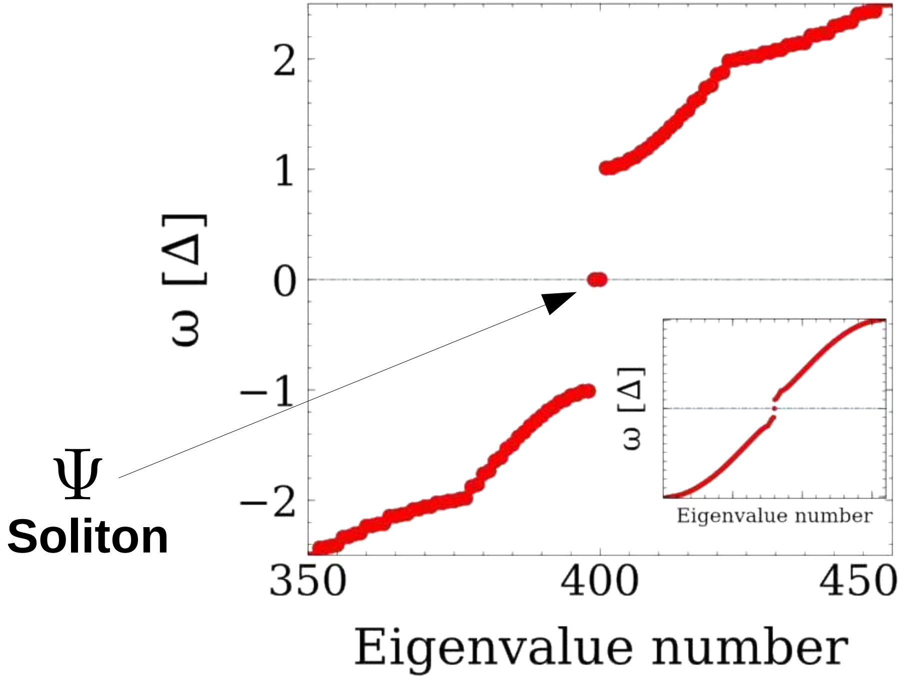
Solitonic in-gap modes appear between the superconductor and the quantum antiferromagnet

Single-particle solitonic zero modes

$$\mathcal{H} = \mathcal{H}_{\mathrm{kin}} + \mathcal{H}_{\mathrm{SC}} + \mathcal{H}_{\mathrm{AF}}$$

Single particle limit (stagger magnetization and no interactions)





In the single-particle limit, solitonic E=0 solutions can be built analytically

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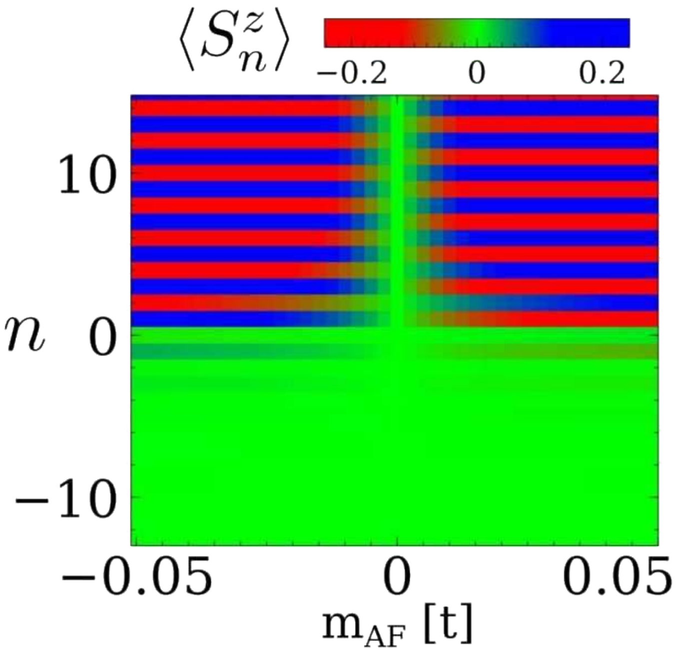
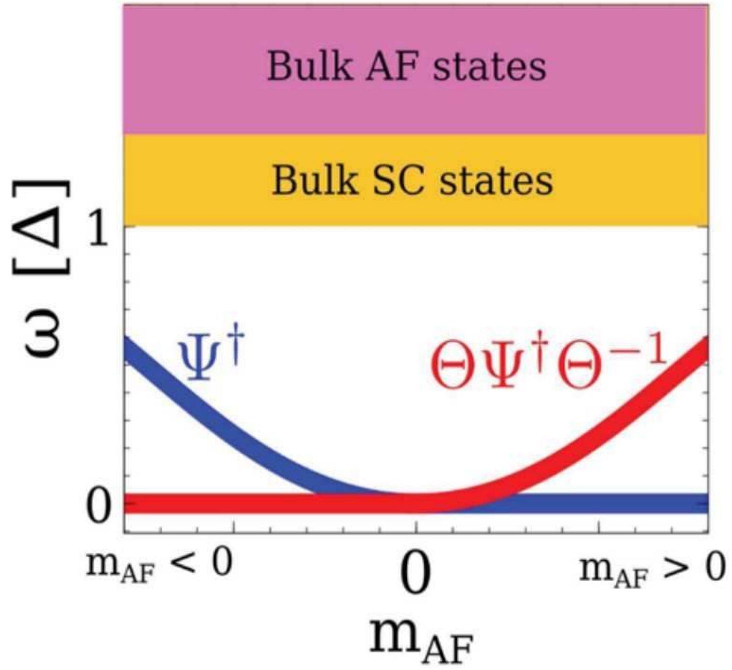
From many-body to the single-particle symmetry broken state

$$\mathcal{H} = \mathcal{H}_{\text{kin}} + \mathcal{H}_{\text{SC}} + \mathcal{H}_{\text{AF}} + \mathcal{H}_{\text{int}}$$

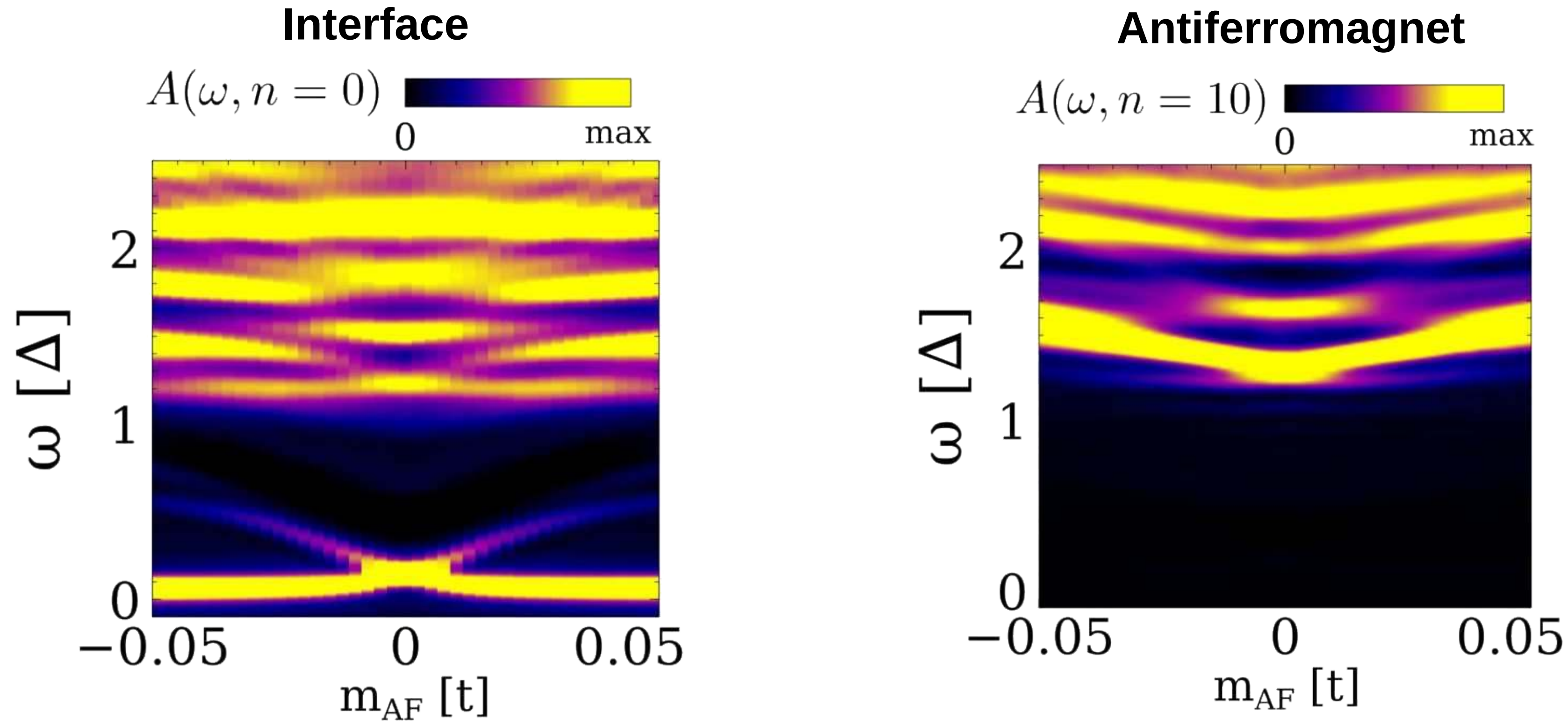


Sketch of the charge excitations



Switching on a magnetization pushes the interacting model to the symmetry broken state

From many-body to symmetry broken



The solitonic single-particle mode transforms into the many-body in-gap mode

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

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

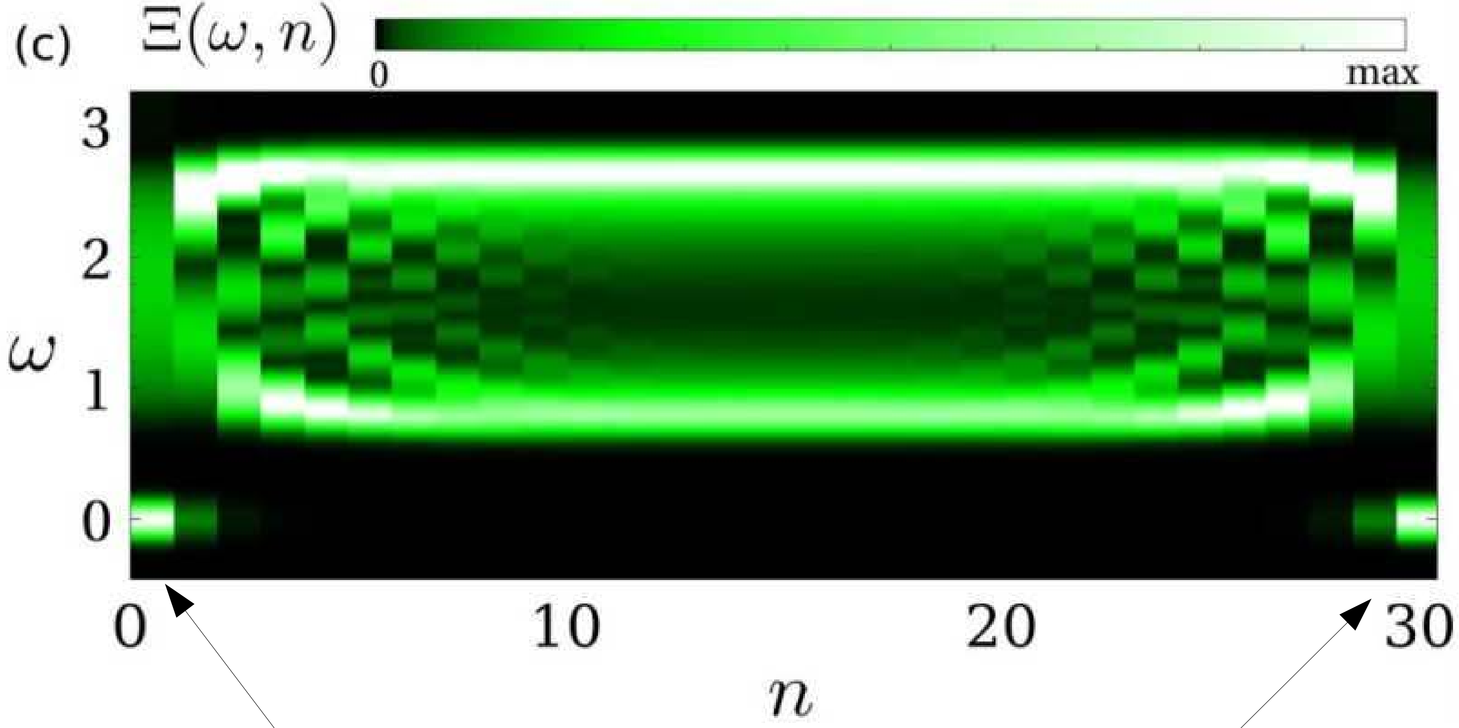
with $\chi_j \psi_k = z \psi_k \chi_j, \quad \chi_j \chi_k = z \chi_k \chi_j, \quad \psi_j \psi_k = z \psi_k \psi_j$

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

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

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

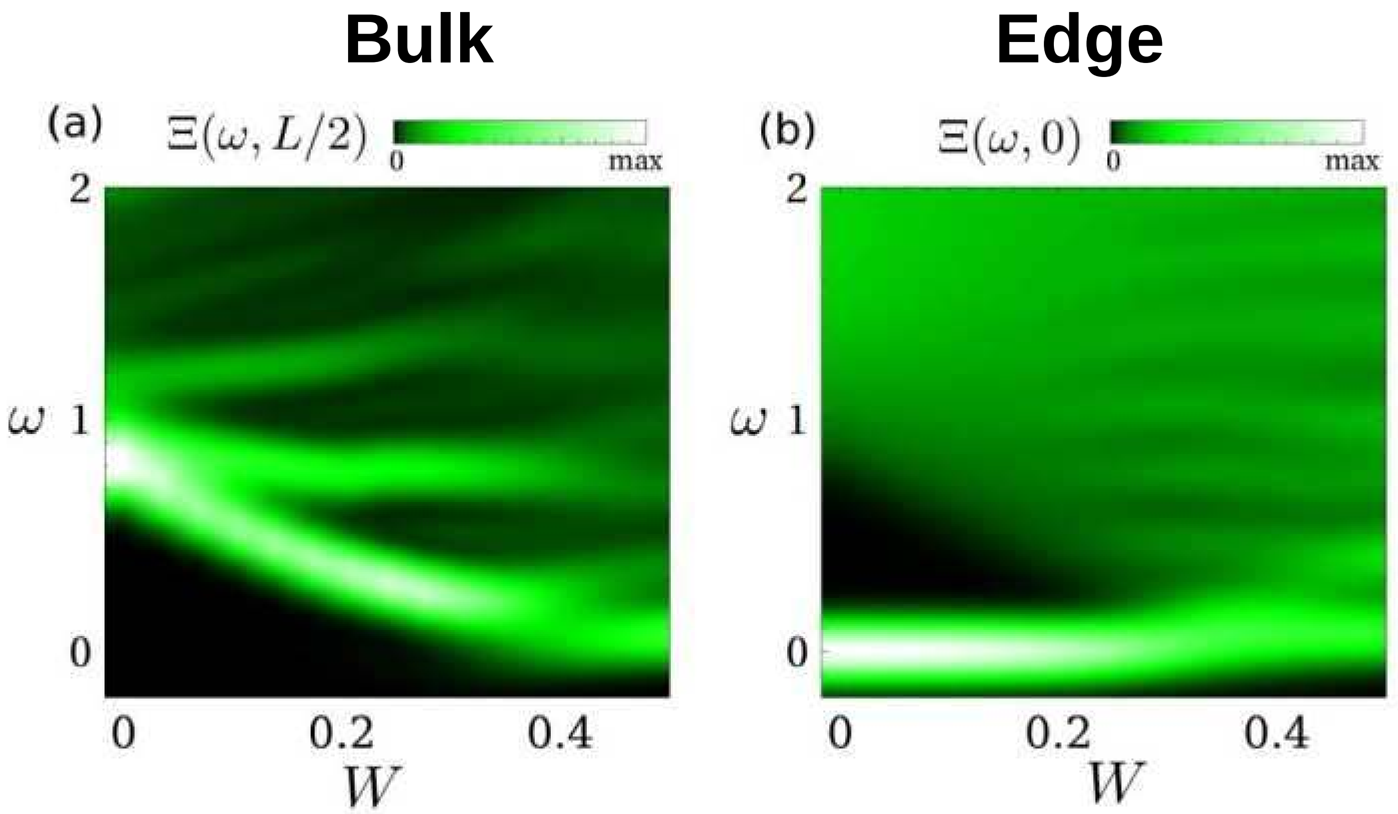
Edge modes in parafermion models



Topological parafermion zero modes

Four-parafermion interactions

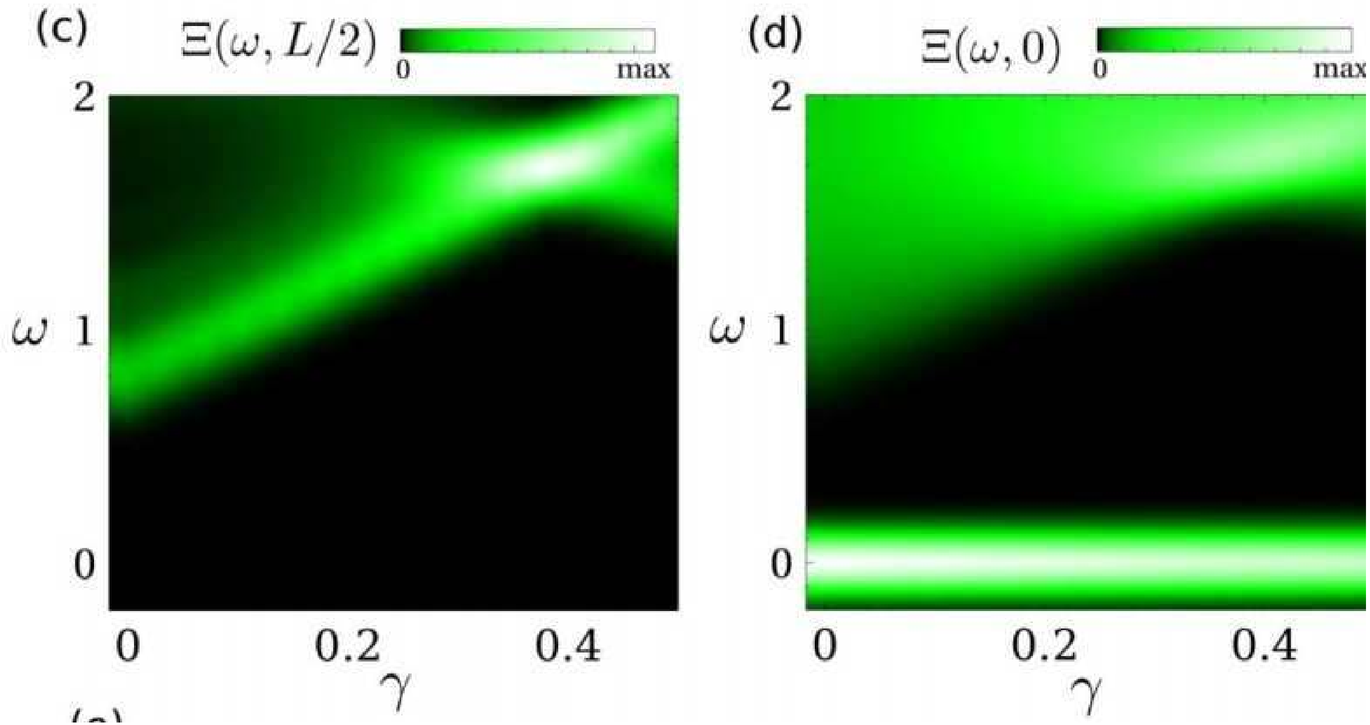
$$W \sum_n \psi_n^\dagger \chi_n \psi_{n+1}^\dagger \chi_{n+1}$$



Zero modes survive in the presence of perturbations

Next-to-nearest neighbor coupling

Bulk **Edge**

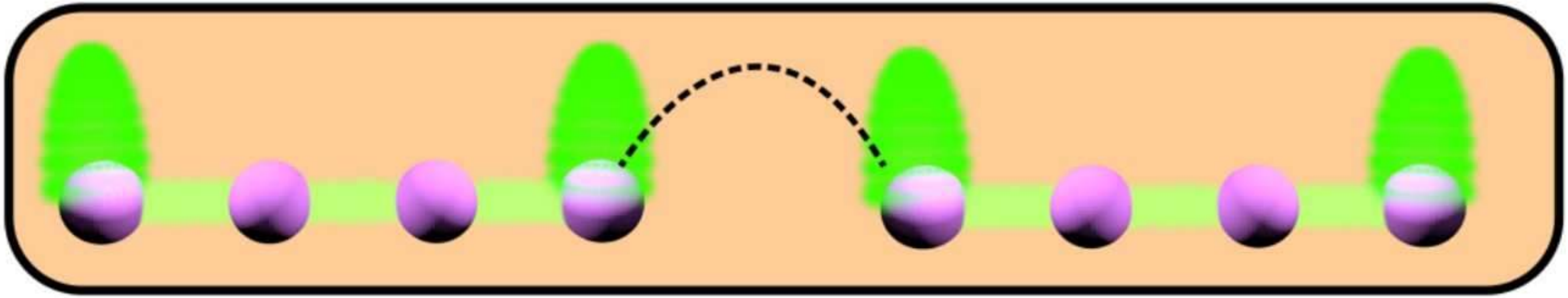


$$-\gamma \sum_n \psi_n^\dagger \chi_{n+2}$$

Zero modes survive in the presence of perturbations

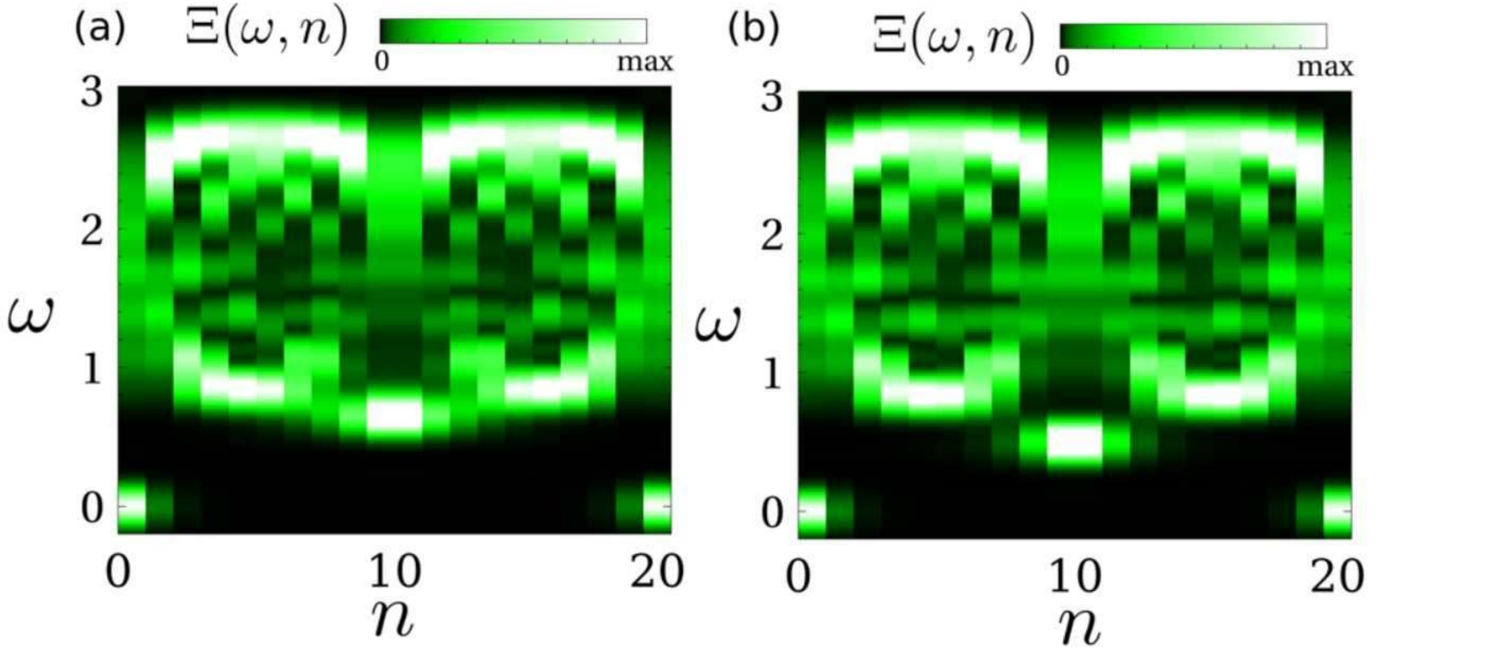
Weakly coupled parafermions

λ



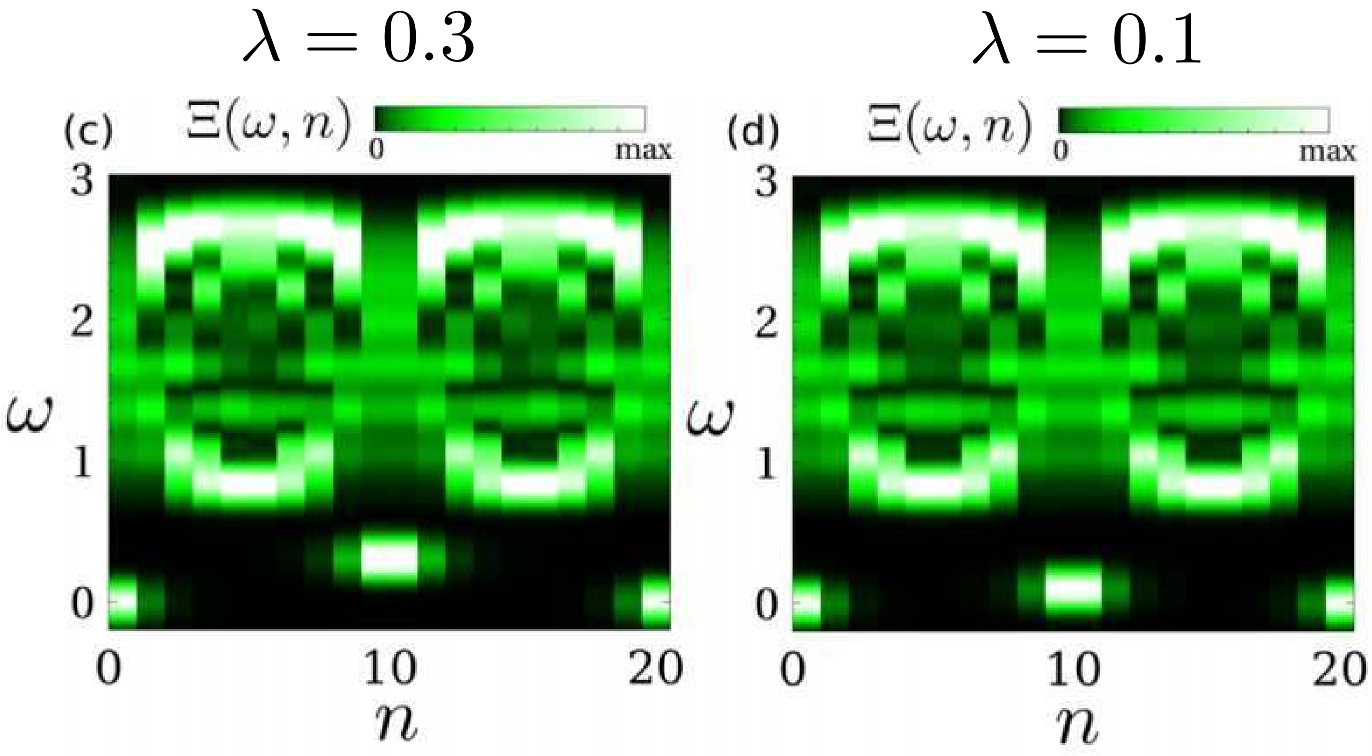
Weakly coupled parafermions

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



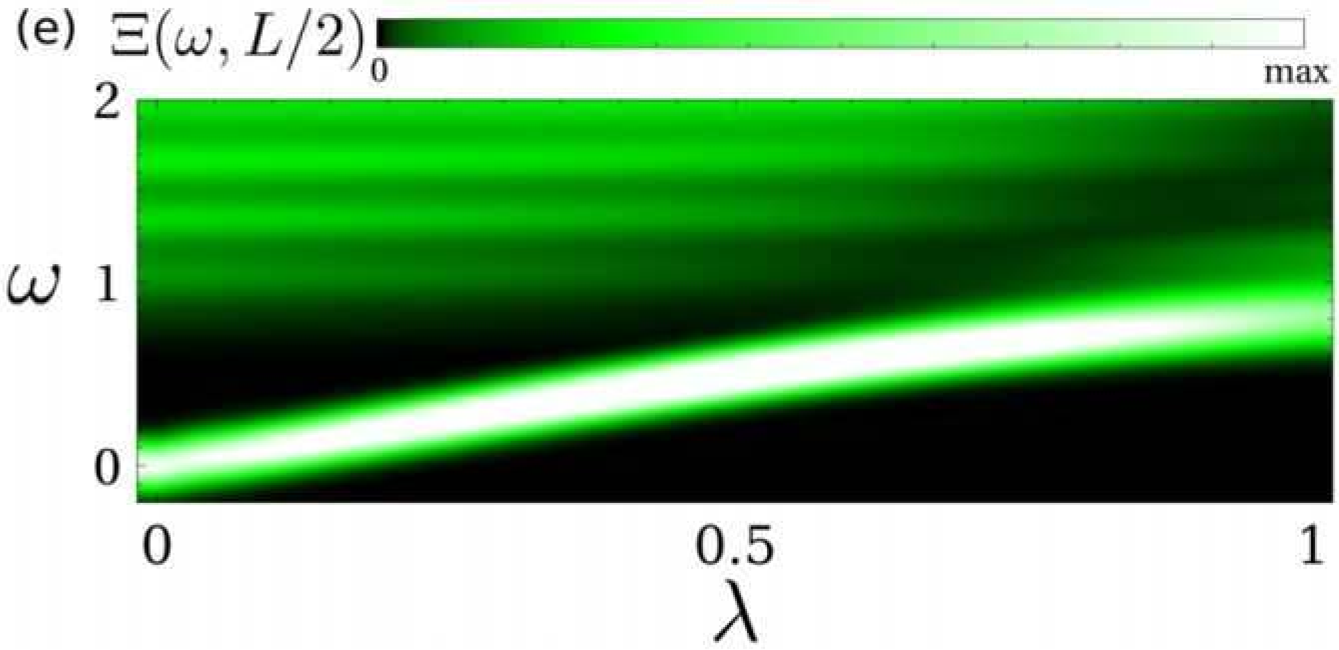
As the chain is decoupled, in-gap parafermion modes appear

Weakly coupled parafermions



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

Open-source software for tensor-network kernel polymonial algorithms

Open-source software for tensor-network kernel polymonial algorithms

dmrgpy

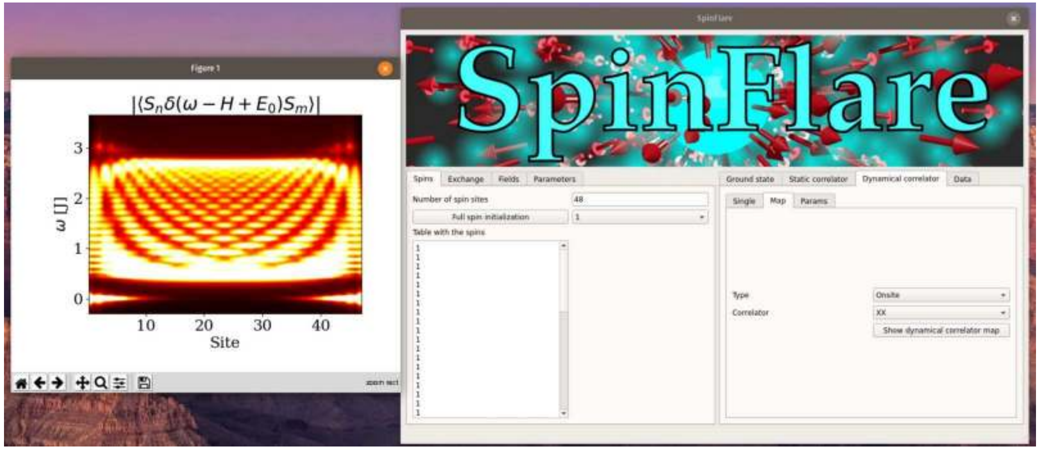
https://github.com/joselado/dmrgpy

```python
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

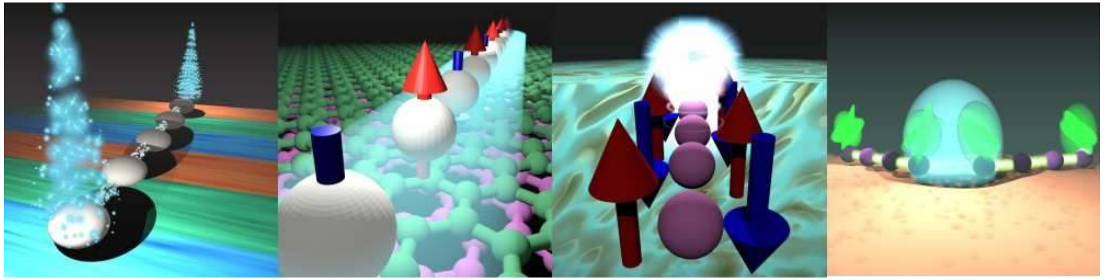


User friendly interface to compute excitations in quantum Heisenberg models

Based on ITENSOR

Take home

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



Thank you!

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