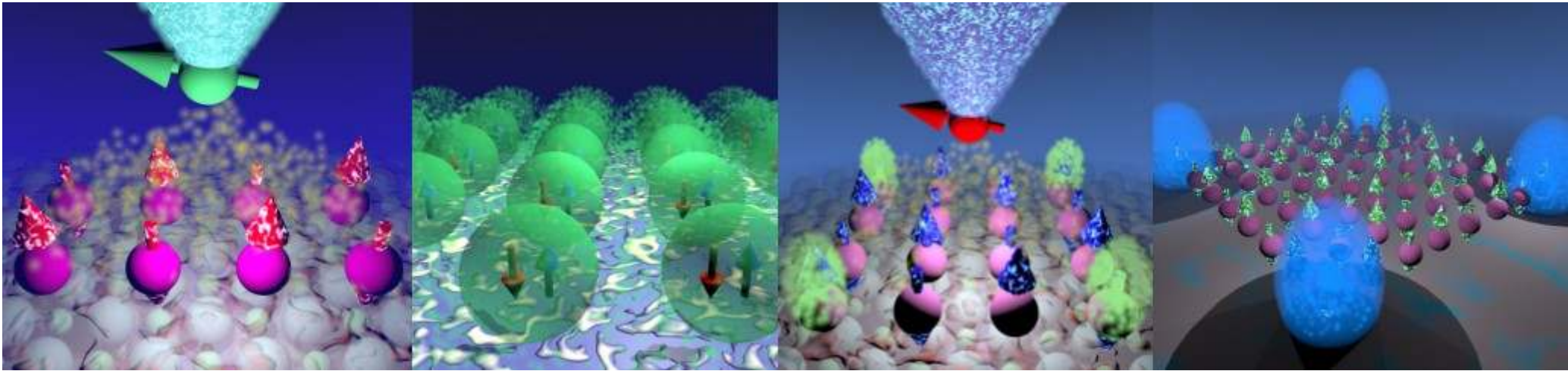


Hamiltonian learning, triplons, and high-order topological order in engineered nanoscale quantum magnets

Jose Lado

Department of Applied Physics, Aalto University, Finland



Phys. Rev. Appl 20, 024054 (2023)

Phys. Rev. Lett. 131, 086701 (2023)

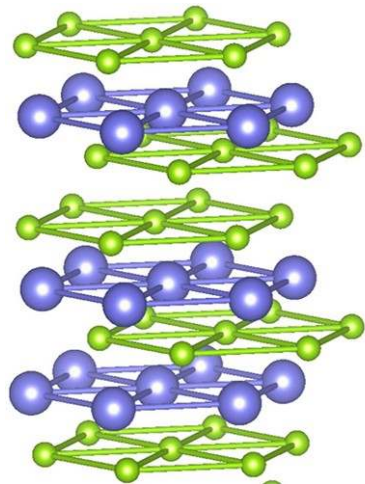
Nature Nano (2024)

arXiv:2408.16453 (2024)

DIPC, Spain, September 30th 2024

Emergence in quantum materials

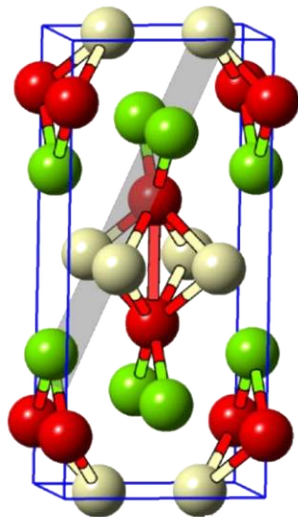
Topological materials



Bi_2Se_3

Science, 325(5937),
178-181 (2009)

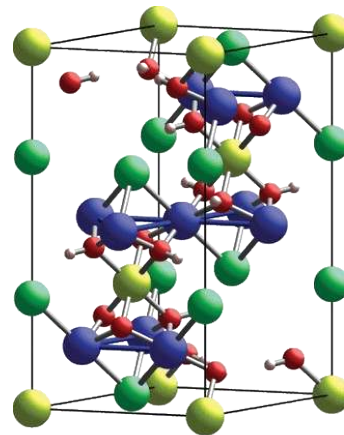
Unconventional superconductors



UTe_2

Nature 579,
523–527 (2020)

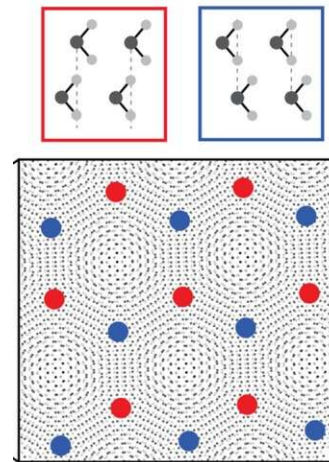
Quantum spin liquids



$\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$

Science 350(6261),
655-658 (2015)

Fractional topological matter

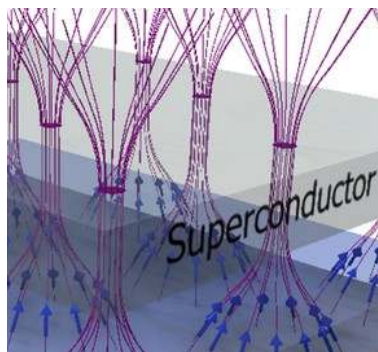


Twisted MoTe_2

Nature (2023)

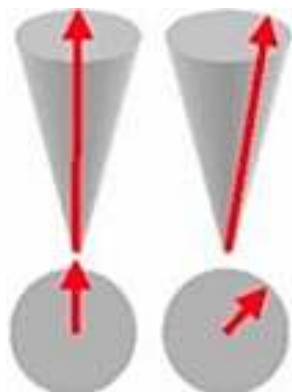
Emergent excitations in quantum materials

Vortexes



Superconductors

Magnons



***Ordered
magnets***

Skyrmions



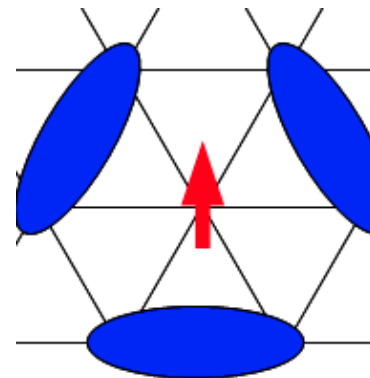
***Non-collinear
magnets***

Dirac fermions



***Topological
materials***

Spinons

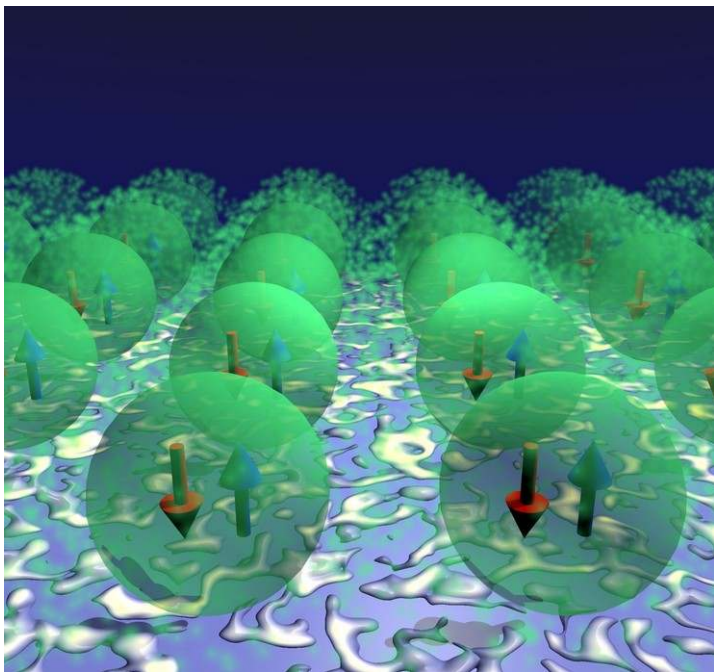


***Quantum spin
liquids***

The discovery of new quasiparticles opens new possibilities in quantum technologies

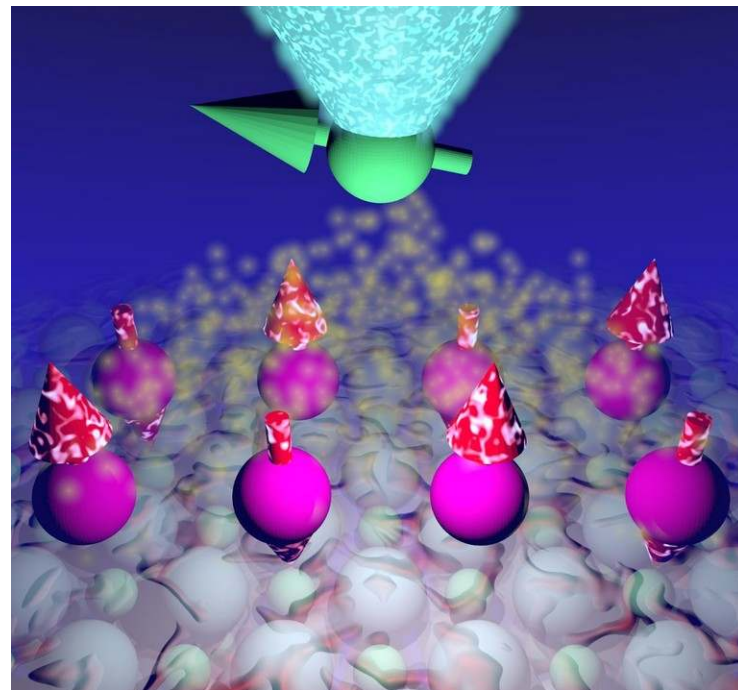
Plan for today

Triplons in a molecular quantum magnet



Phys. Rev. Lett. 131, 086701 (2023)

Hamiltonian learning nanoscale magnets



Phys. Rev. Applied 20, 024054 (2023)

Behind the scenes

Triplons in a molecular quantum magnet

Robert Drost



Shawulienu Kezilebieke



Peter Liljeroth



Phys. Rev. Lett. 131, 086701 (2023)

Hamiltonian learning nanoscale magnets

Netta Karjalainen



Zina Lippo



Rouven Koch



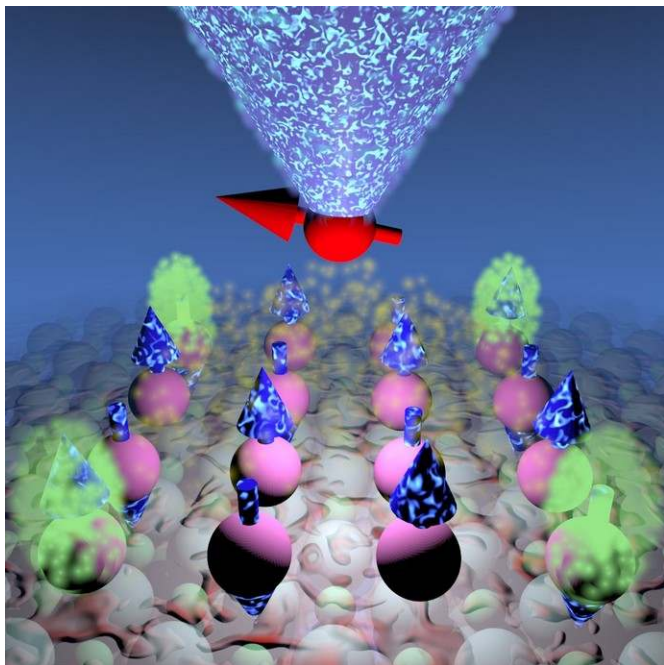
Guangze Chen Adolfo Fumega



Phys. Rev. Applied 20, 024054 (2023)

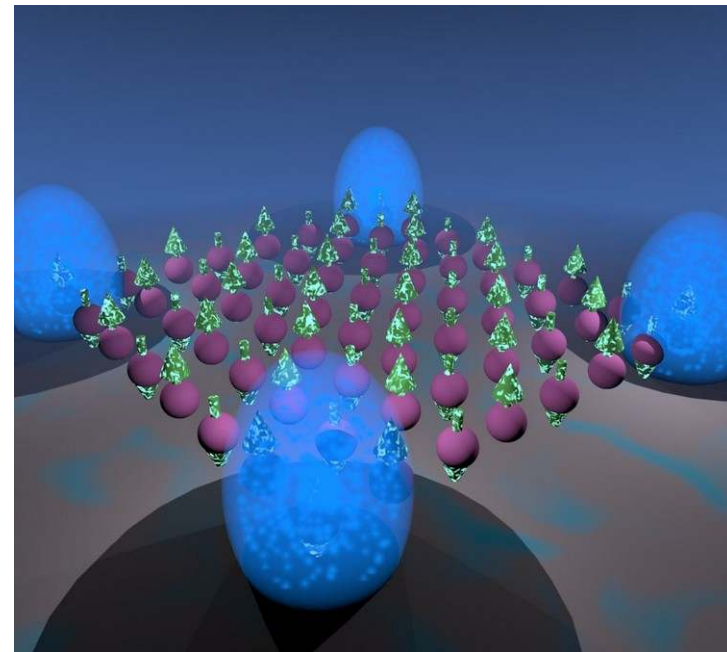
Plan for today

Realization of a higher order topological quantum magnet



Nature Nanotechnology (2024), 10.1038/s41565-024-01775-2

Phase diagram of the higher order topological quantum magnet



arXiv:2408.16453 (2024)

Behind the scenes

Realization of a higher order topological quantum magnet

Hao Wang



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Peng Fang



Hong-Jun Gao



Kai Yang



Nature Nanotechnology (2024), 10.1038/s41565-024-01775-2

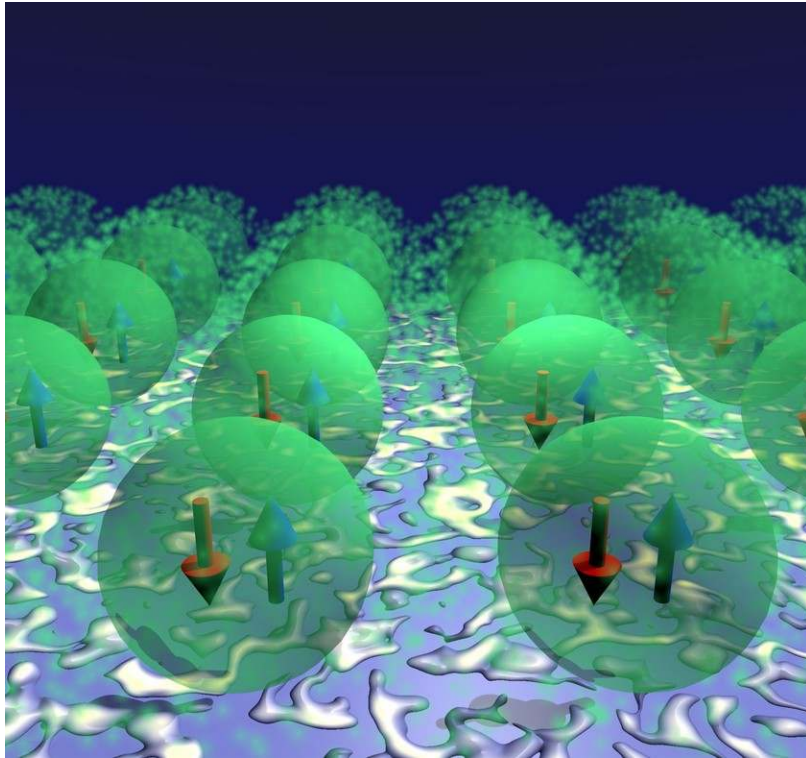
Phase diagram of the higher order topological quantum magnet

Pascal Vecsei



arXiv:2408.16453 (2024)

Triplons in an artificial molecular quantum magnet



Phys. Rev. Lett. 131, 086701 (2023)

Triplons in an atomic-scale quantum magnet

Robert Drost



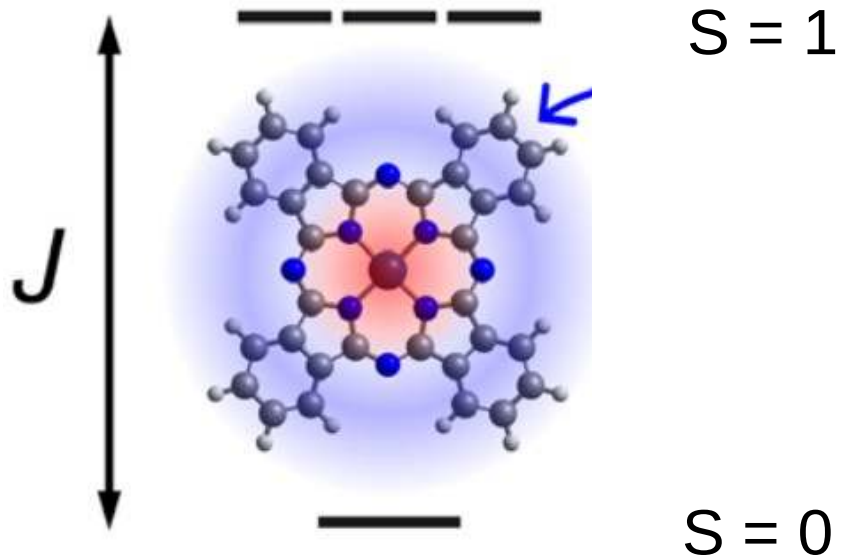
Shawulienu Kezilebieke



Peter Liljeroth



Triplet excitations in a molecule

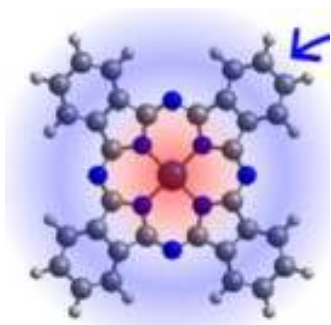


Internal antiferromagnetic coupling

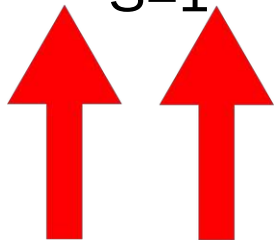
$$H = JS \cdot \mathbf{K}$$

A single molecule (CoPC) has a singlet-triplet transition

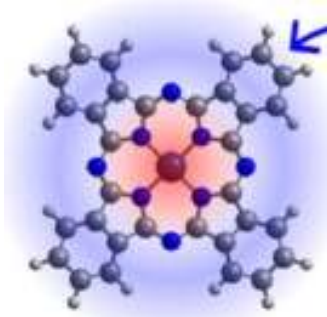
Triplons in a dimer



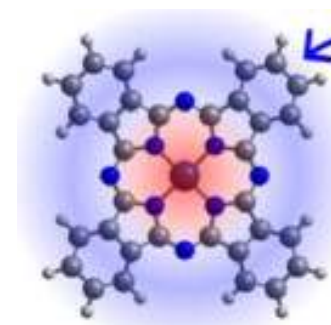
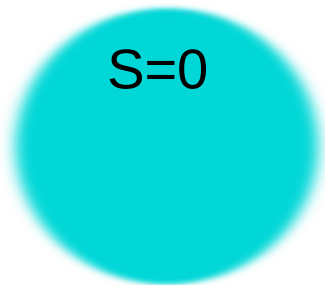
$S=1$



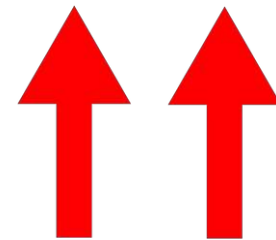
A triplet in the first molecule



$S=0$



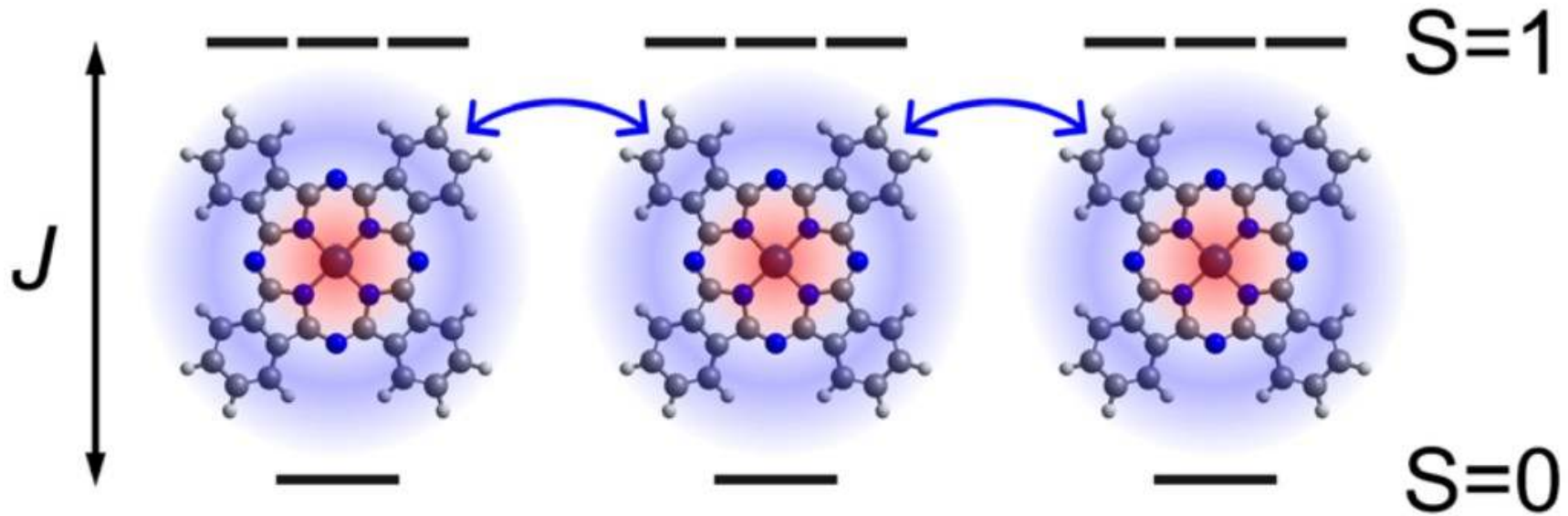
$S=1$



Can jump to the second molecule

Exchange coupling between molecules leads to propagating triplon excitations

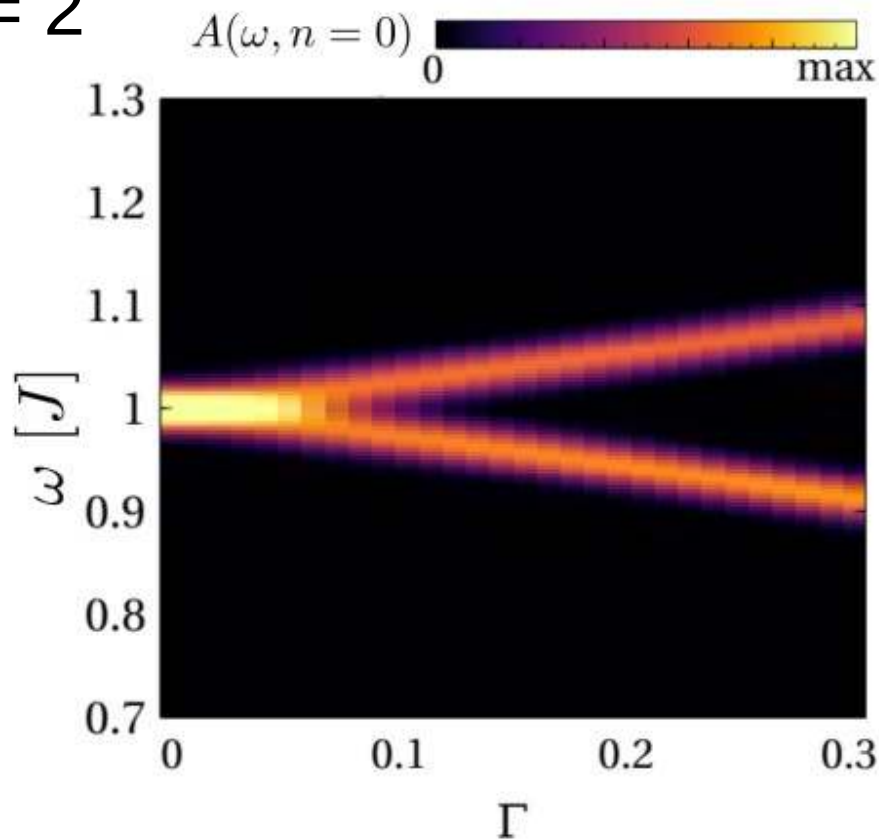
A chain of triplons



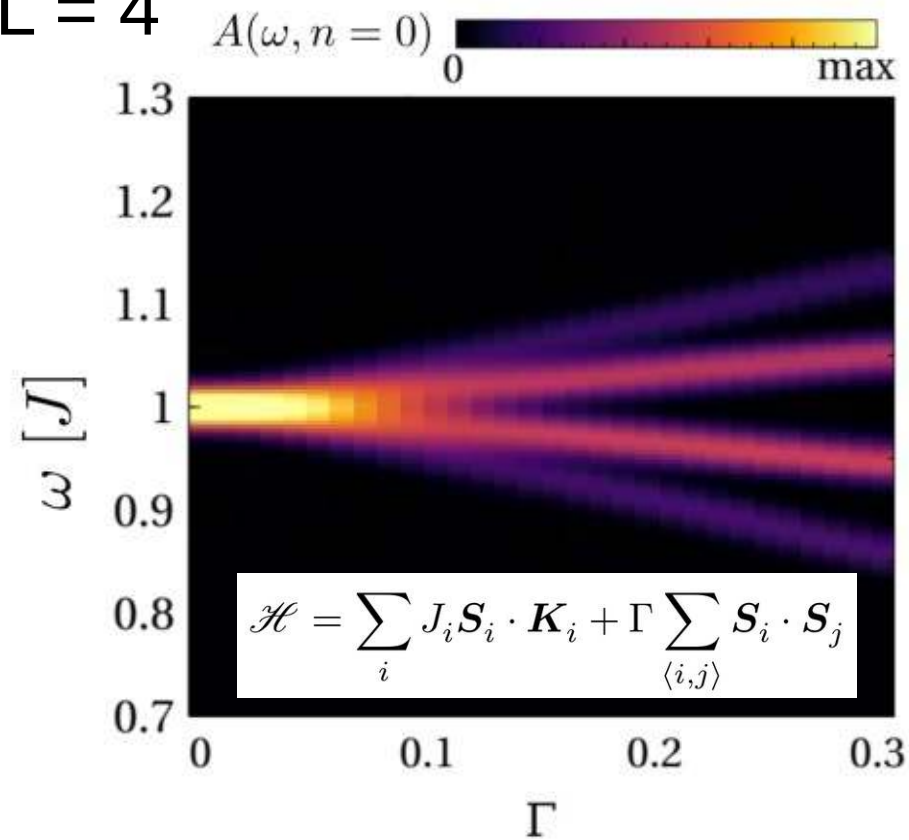
$$\mathcal{H} = \sum_i J_i \mathbf{S}_i \cdot \mathbf{K}_i + \Gamma \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

Chains of triplons

$L = 2$

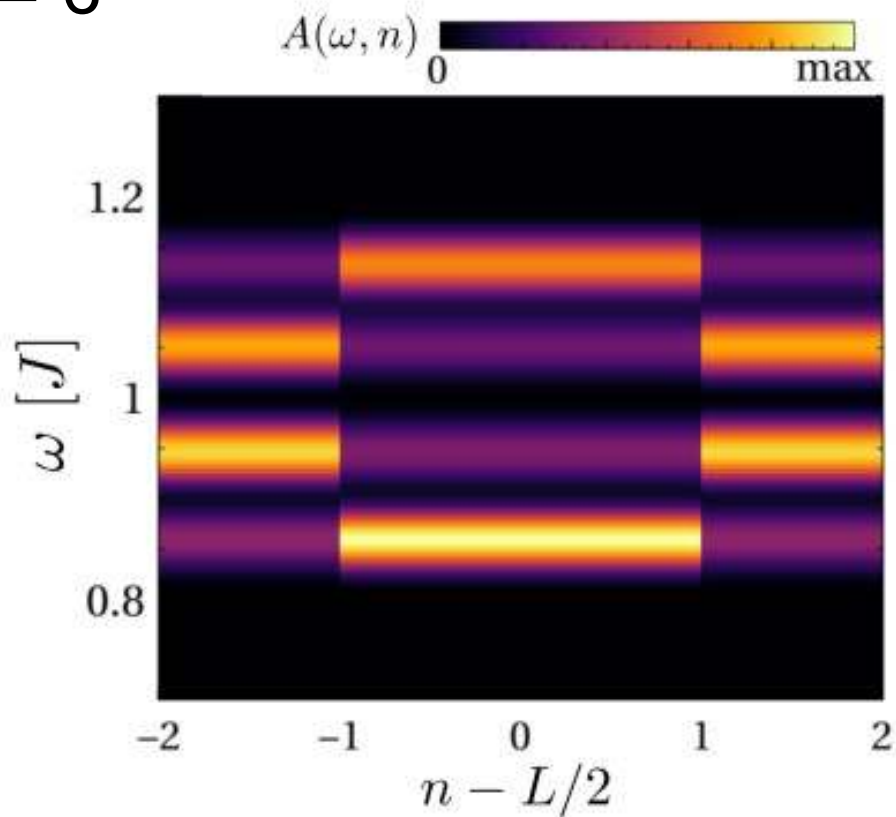


$L = 4$

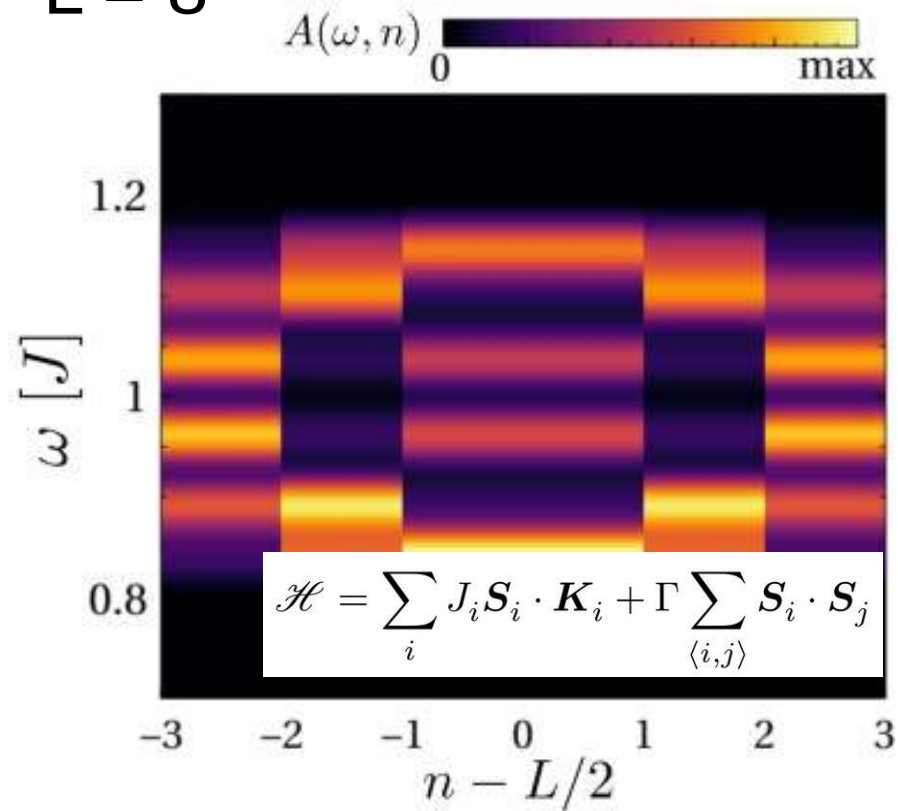


Chains of triplons

$L = 6$



$L = 8$



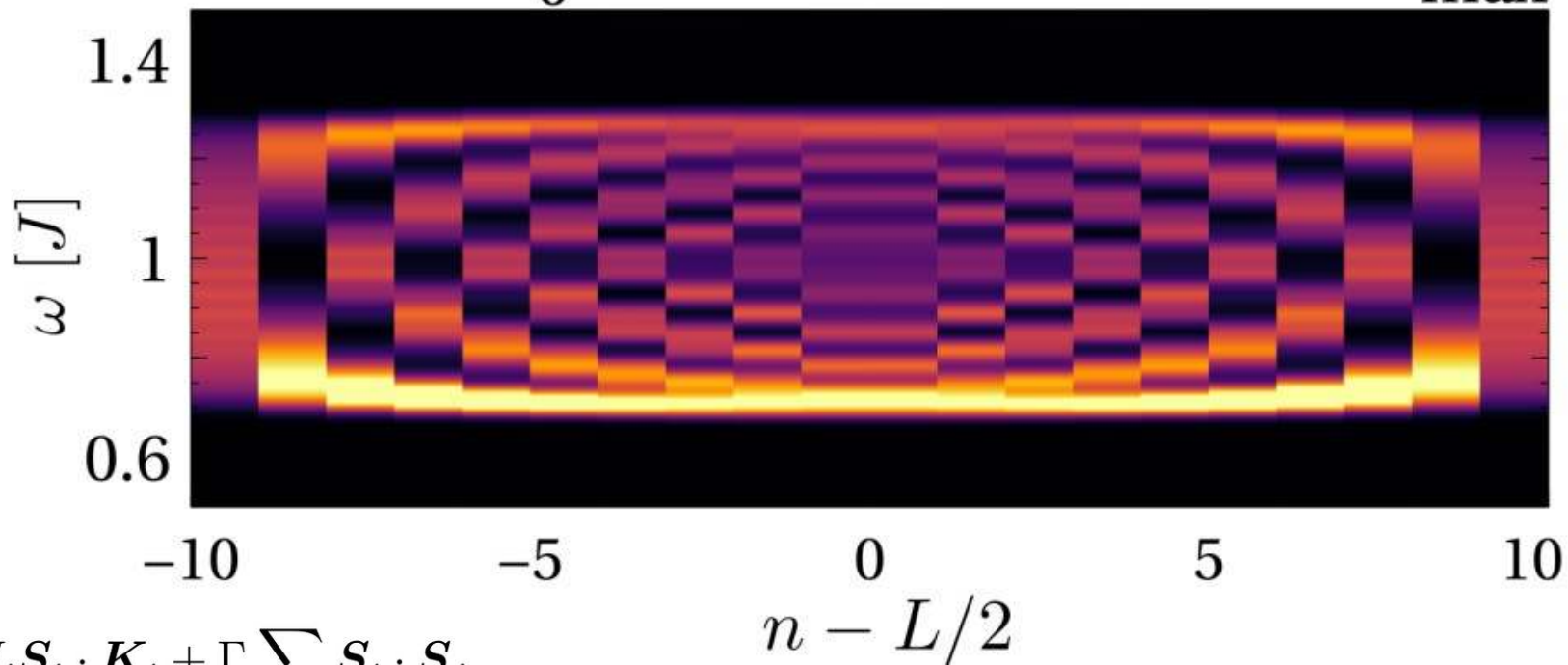
Chains of triplons

$L = 20$

$A(\omega, n)$

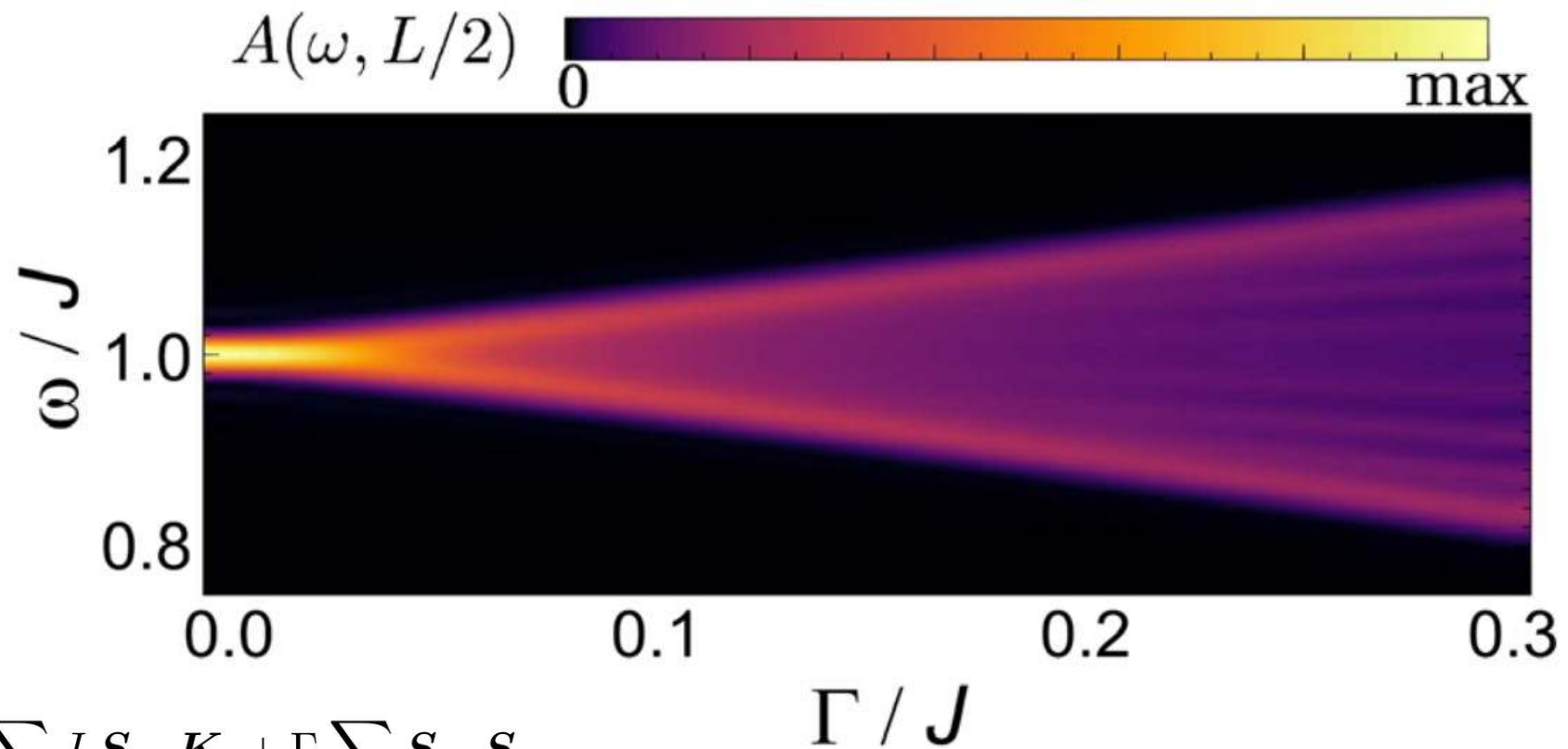


0 max



$$\mathcal{H} = \sum_i J_i \mathbf{S}_i \cdot \mathbf{K}_i + \Gamma \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

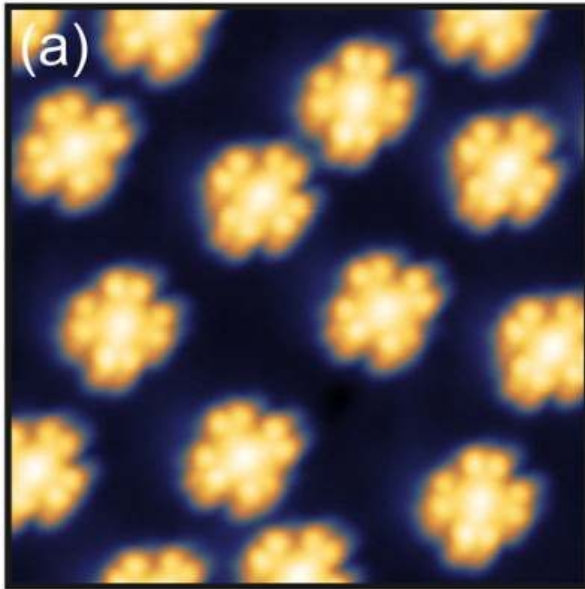
Chains of triplons



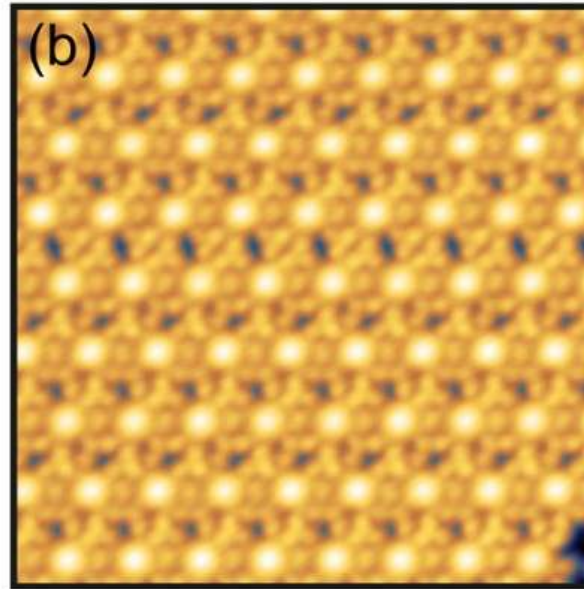
$$\mathcal{H} = \sum_i J_i \mathbf{S}_i \cdot \mathbf{K}_i + \Gamma \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

0D, 1D and 2D arrays

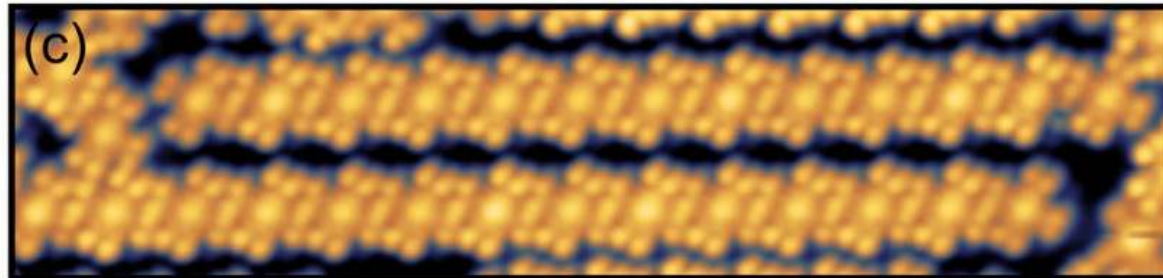
0D



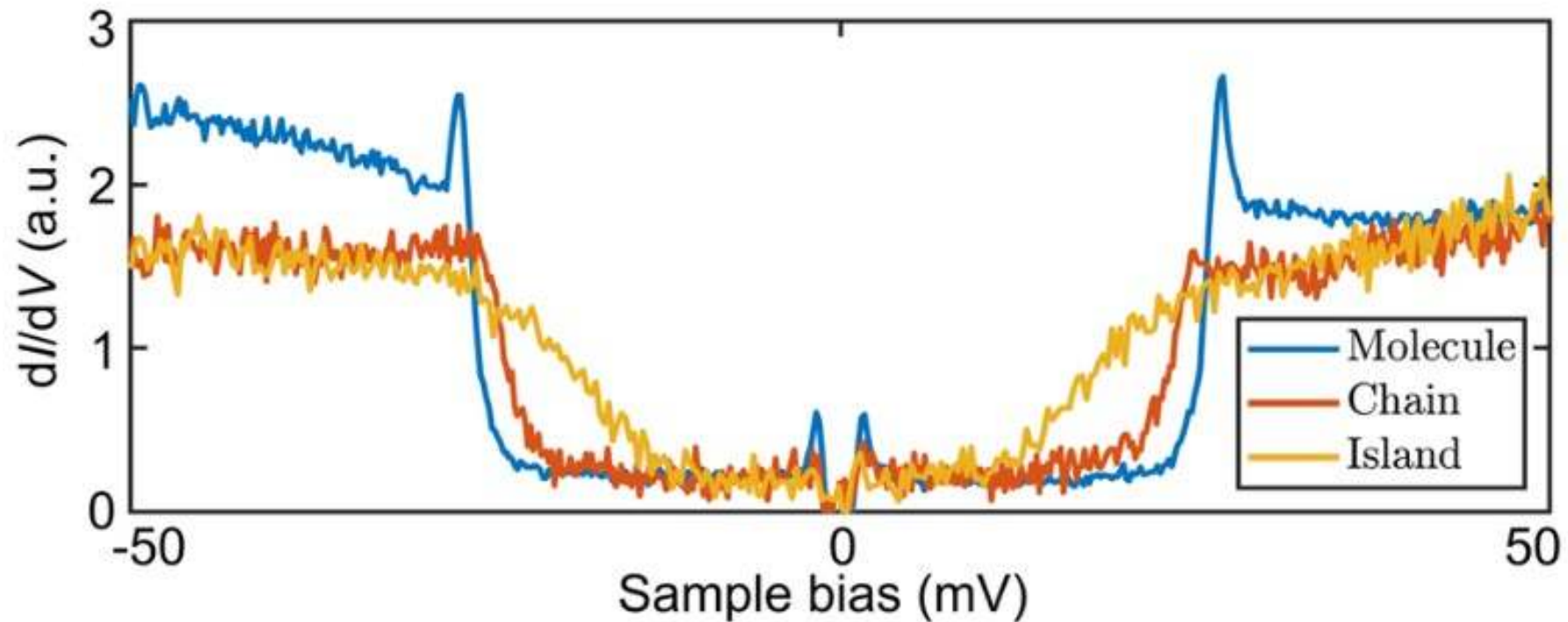
2D



1D

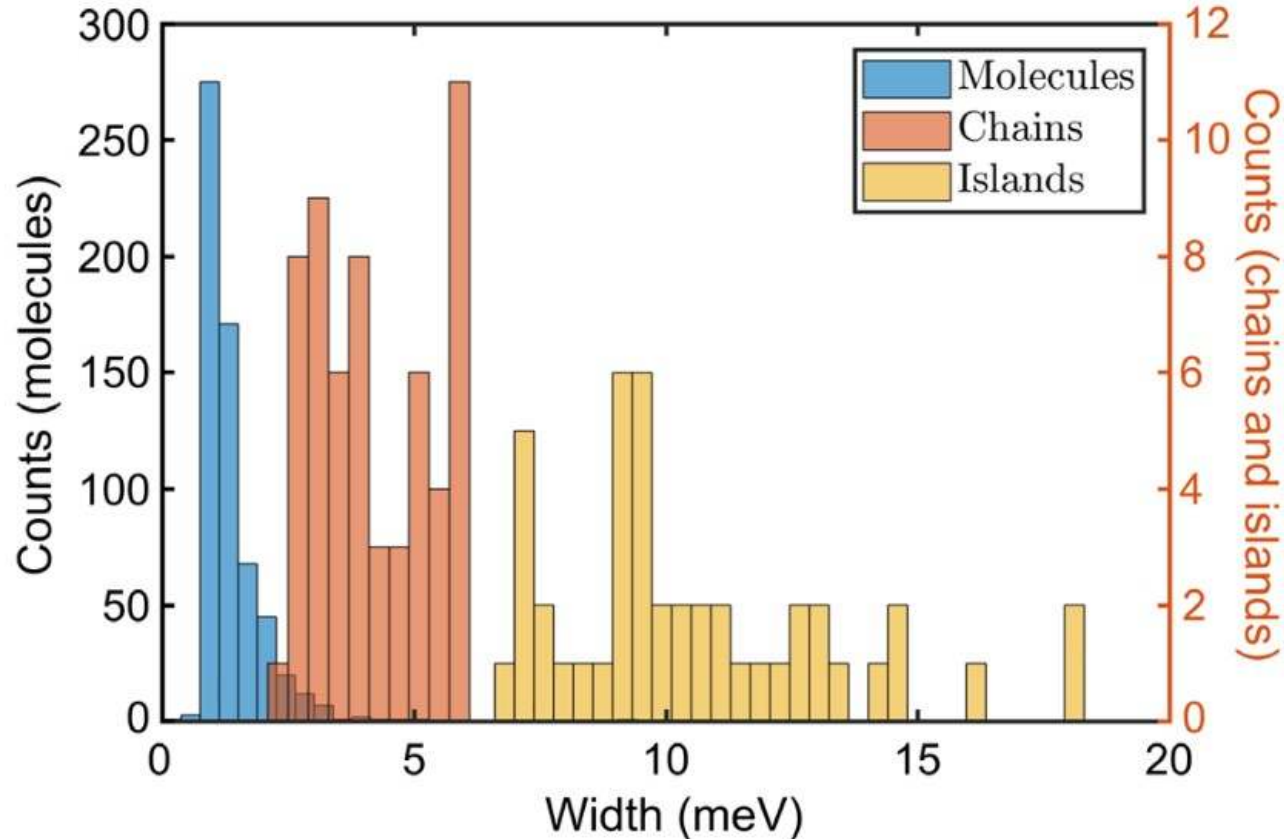


Inelastic excitations for 0D, 1D and 2D arrays



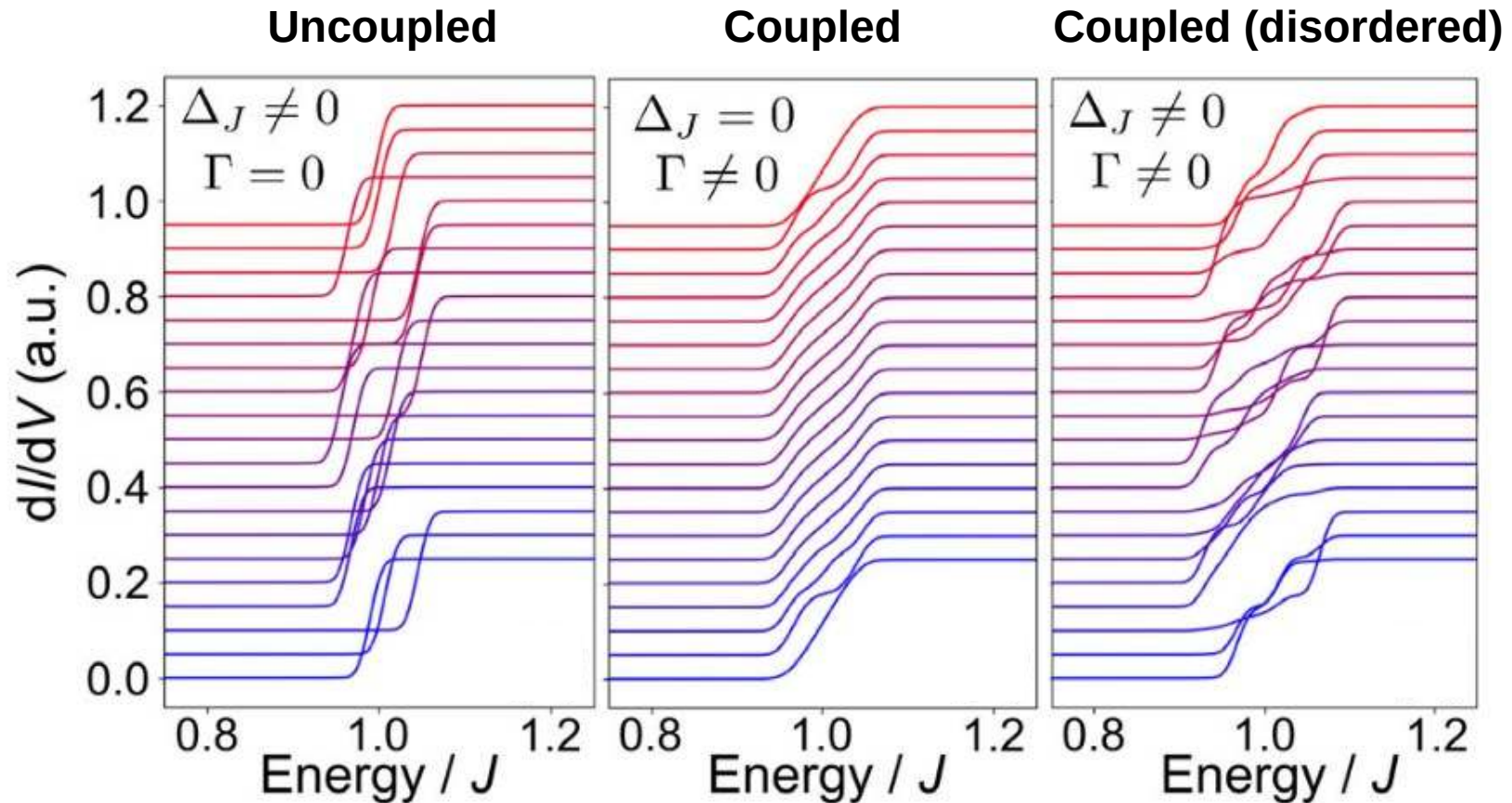
The width of the step is bigger for islands than for molecules

Statistic of the inelastic steps

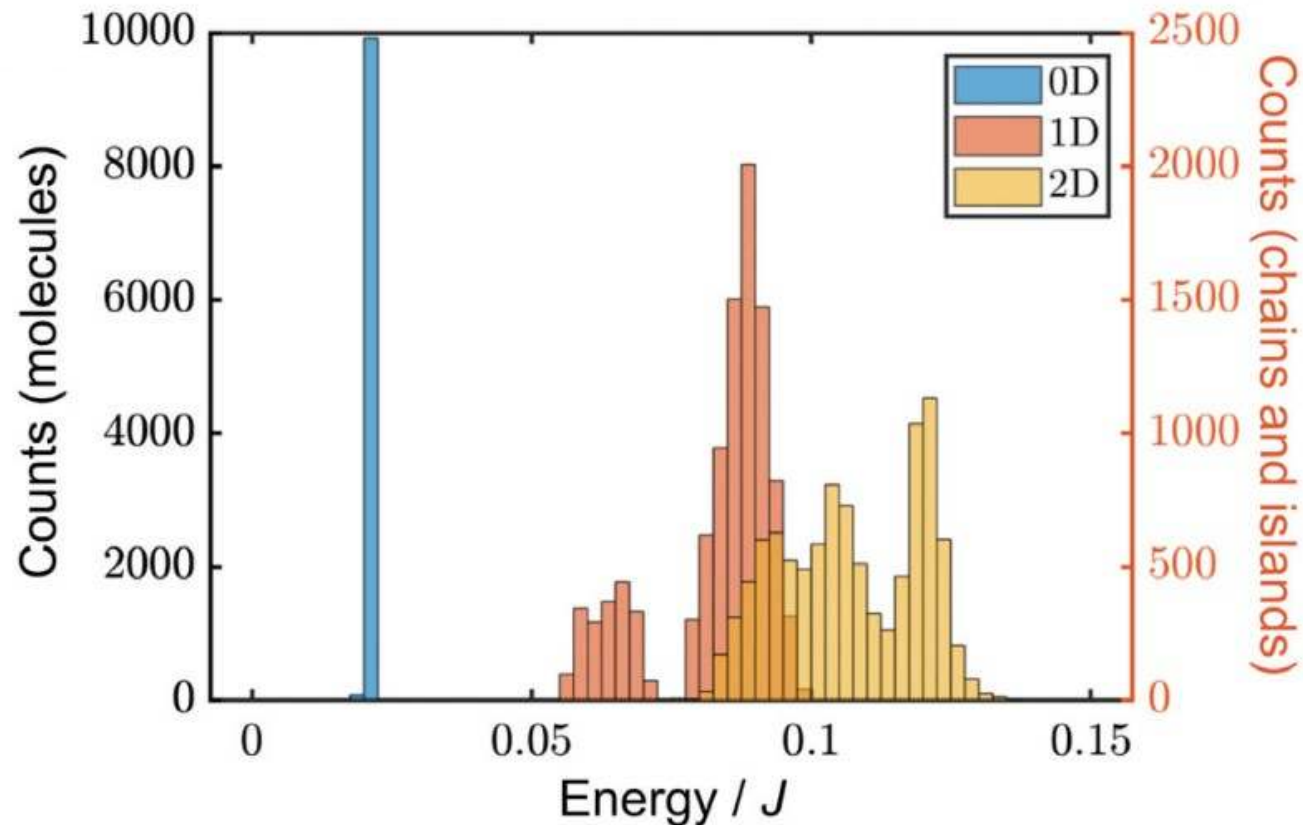


2D arrays have the largest width of the spin excitation

Coupled and uncoupled inelastic excitation

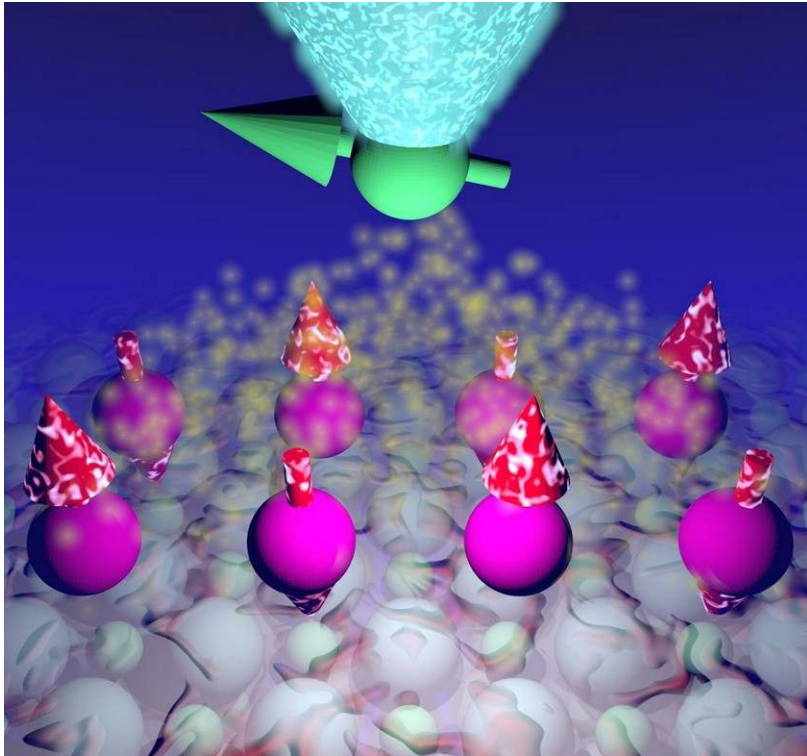


Statistics of the theoretical model



2D arrays have the largest width of the spin excitation

Hamiltonian learning nanoscale magnets



Hamiltonian learning nanoscale magnets

Netta Karjalainen

Zina Lippo



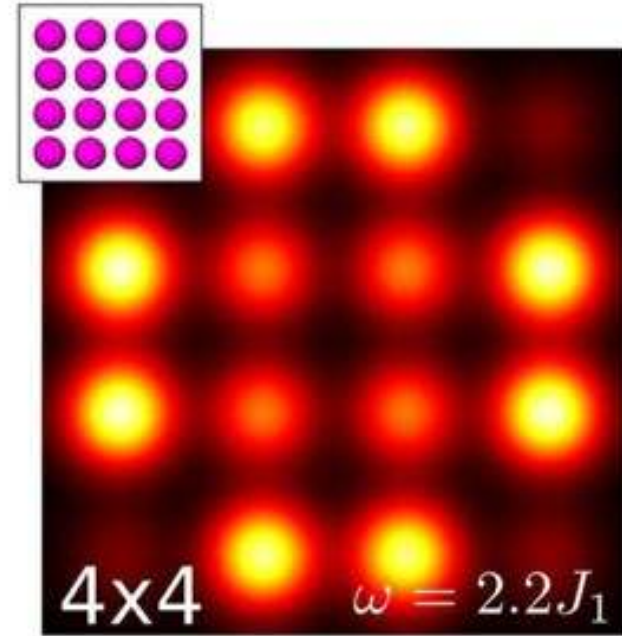
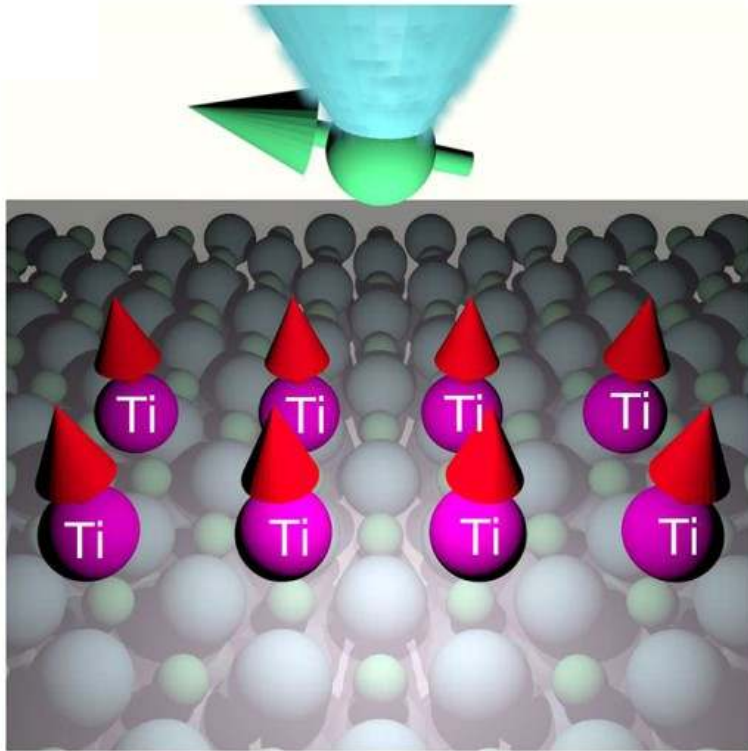
Rouven Koch

Guangze Chen Adolfo Fumega



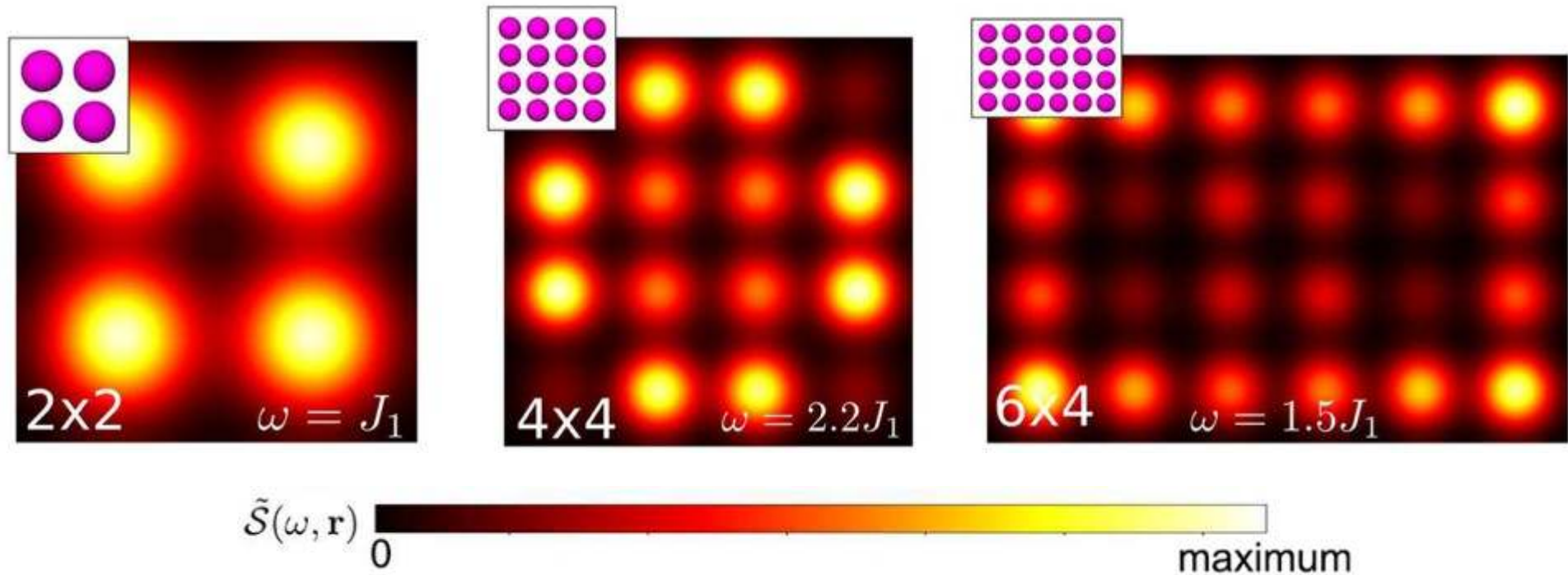
Phys. Rev. Applied 20, 024054 (2023)

Spatially resolved excitations



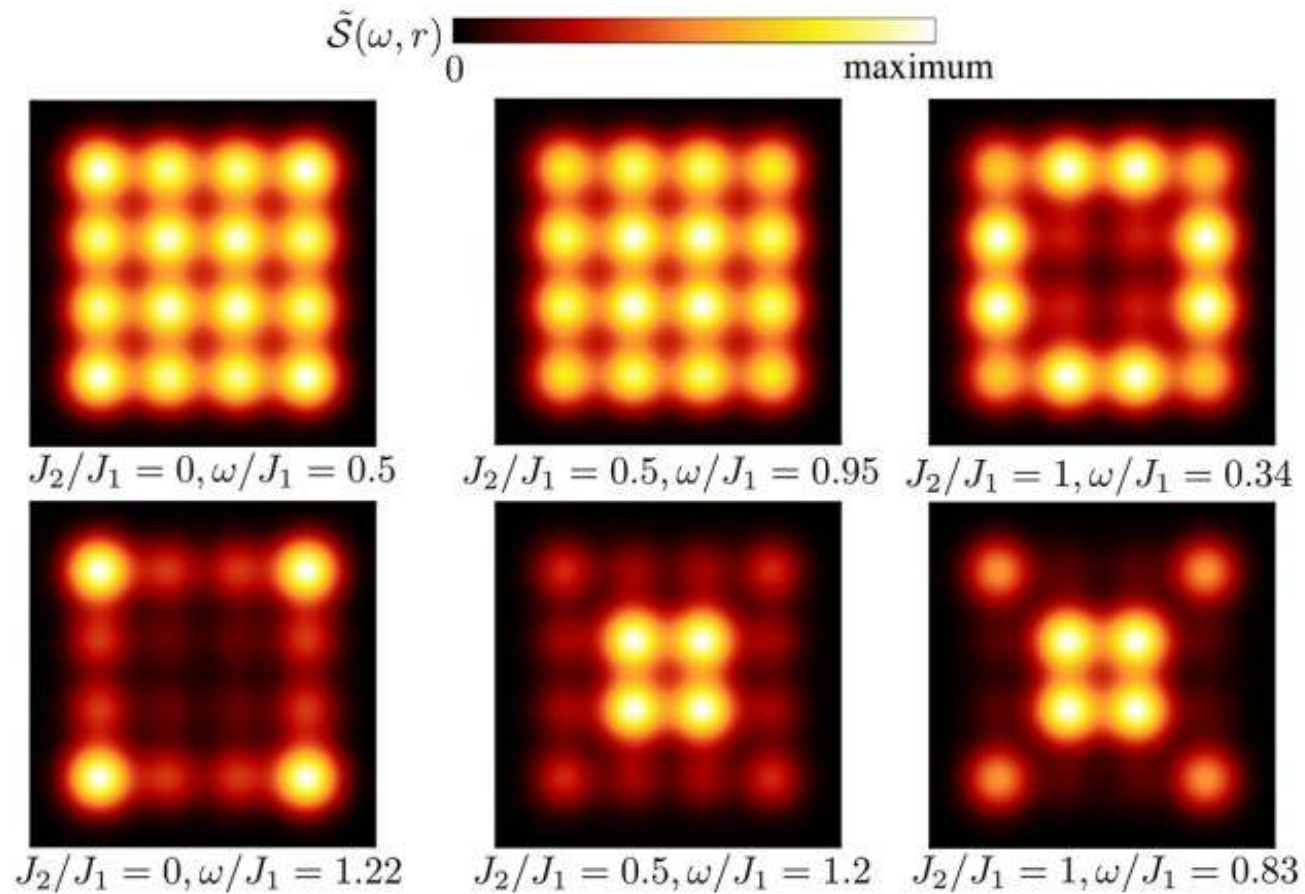
What can we learn from the Hamiltonian using real-space information?

Spatially resolved excitations



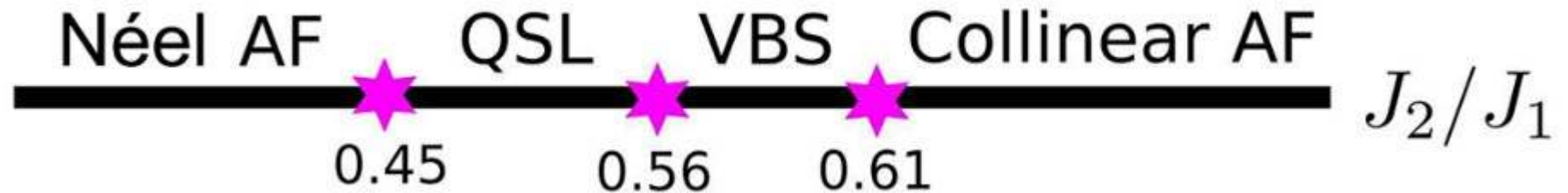
Spin excitations behave like particle in a box states

Spin excitation modes in spin islands



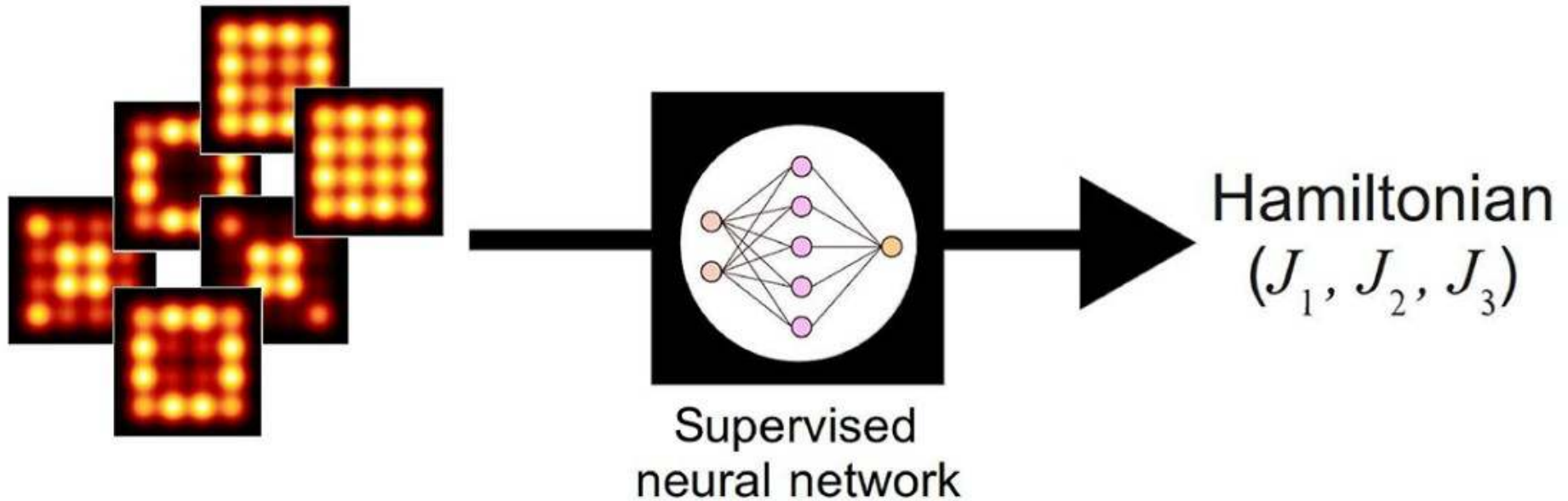
The extended Heisenberg model

$$\mathcal{H} = J_1 \sum_{\langle \mathbf{r}_i, \mathbf{r}_j \rangle} \mathbf{S}_{\mathbf{r}_i} \cdot \mathbf{S}_{\mathbf{r}_j} + J_2 \sum_{\langle\langle \mathbf{r}_i, \mathbf{r}_j \rangle\rangle} \mathbf{S}_{\mathbf{r}_i} \cdot \mathbf{S}_{\mathbf{r}_j}$$



Can we learn the exchange couplings from atomic-scale spin islands?

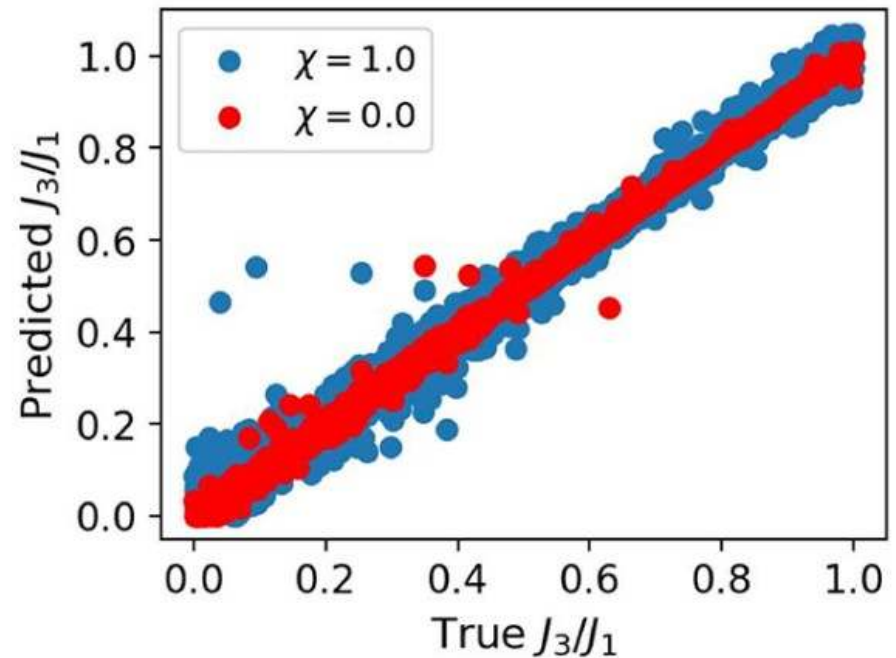
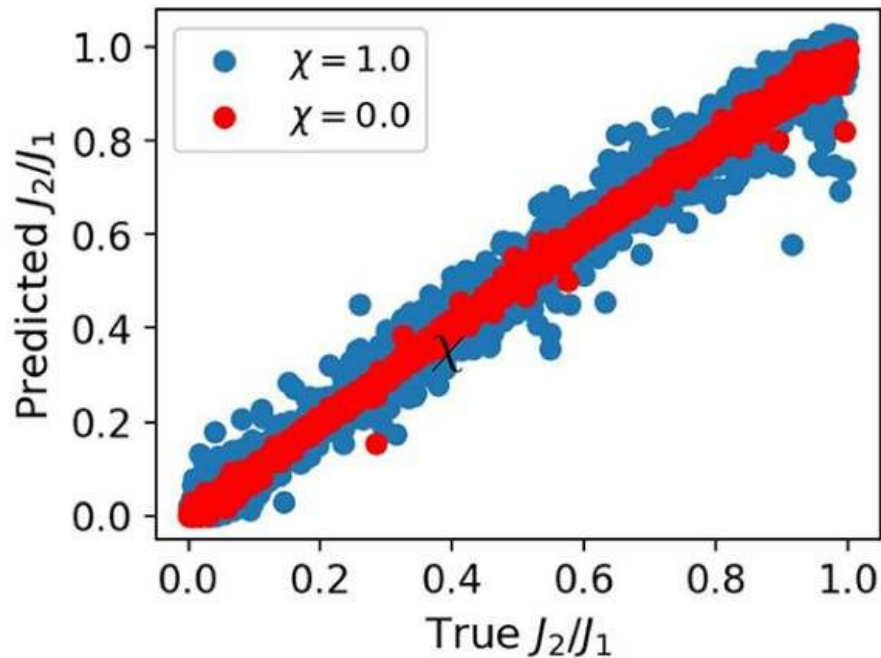
The idea of Hamiltonian learning



Provide the spectroscopy as input, obtain the Hamiltonian as output

Real VS predicted exchange parameters

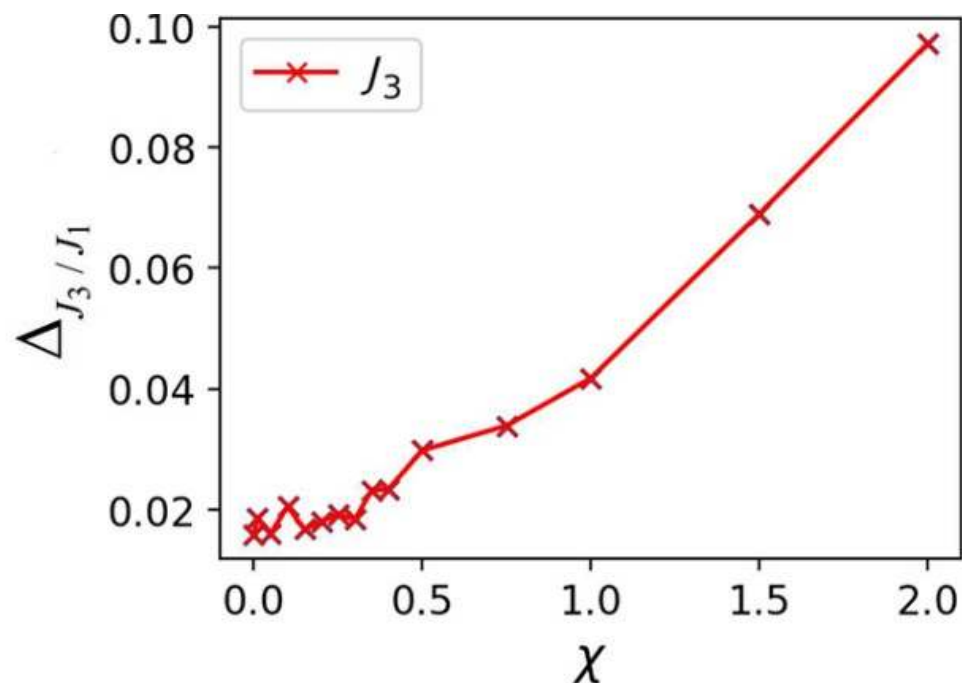
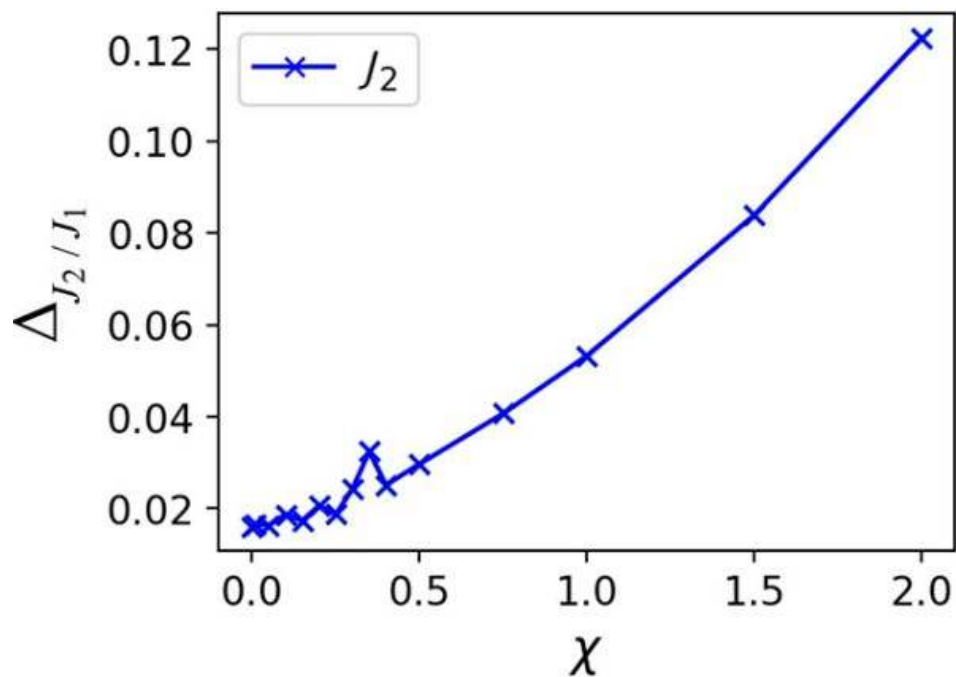
With noise $\mathcal{S}(\omega, \mathbf{r}_i)_{\text{noisy}} = \mathcal{S}(\omega, \mathbf{r}_i) \cdot |1 + \zeta(\omega)| \quad \zeta(\omega) \in [-\chi, \chi]$



A supervised learning algorithm extracts faithfully the exchange parameters

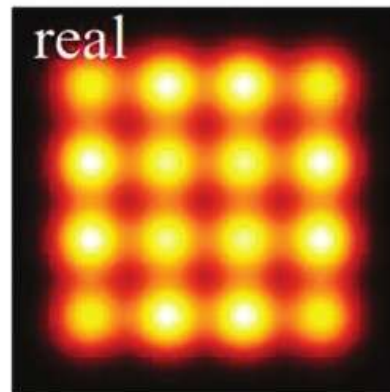
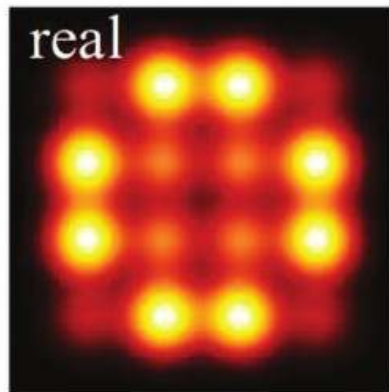
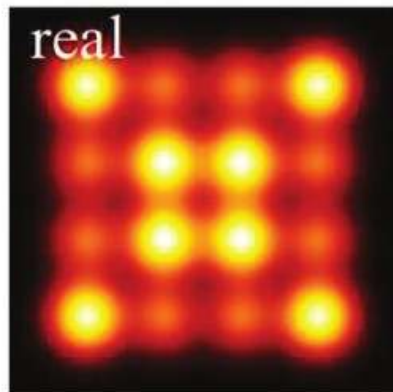
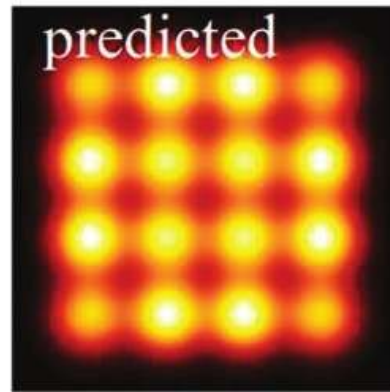
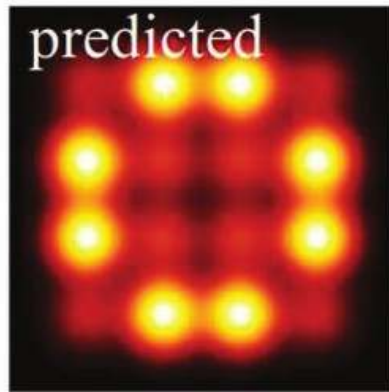
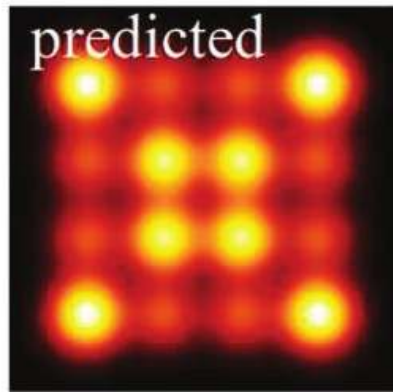
Predictions with noise

$$\mathcal{S}(\omega, \mathbf{r}_i)_{\text{noisy}} = \mathcal{S}(\omega, \mathbf{r}_i) \cdot |1 + \zeta(\omega)| \quad \zeta(\omega) \in [-\chi, \chi]$$

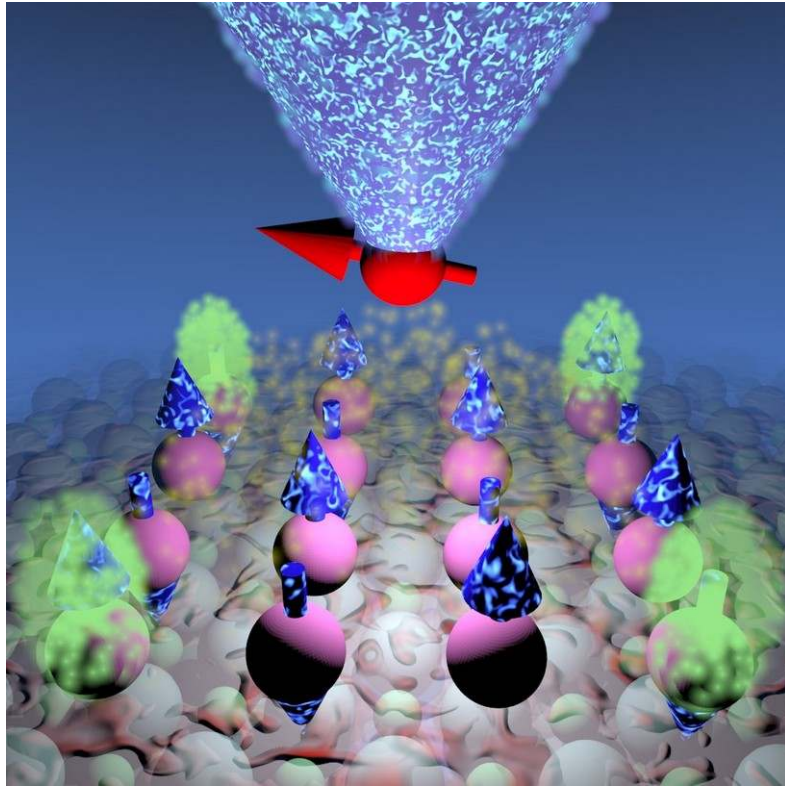


Quality of prediction remain good with sizable noise levels

Predicted VS real spin excitations



Engineering a higher order topological quantum magnet



Hao Wang



Jing Chen



Lili Jiang



Peng Fang



Hong-Jun Gao



Kai Yang



Nature Nanotechnology (2024)

10.1038/s41565-024-01775-2

Topological quantum magnets

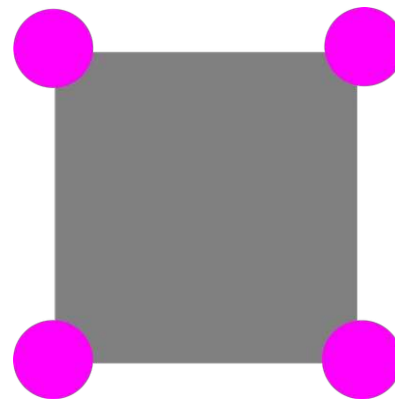
First order topological quantum magnet



1D gaped bulk
0D fractional edge modes

Nature 598, 287–292 (2021)

Second order topological quantum magnet



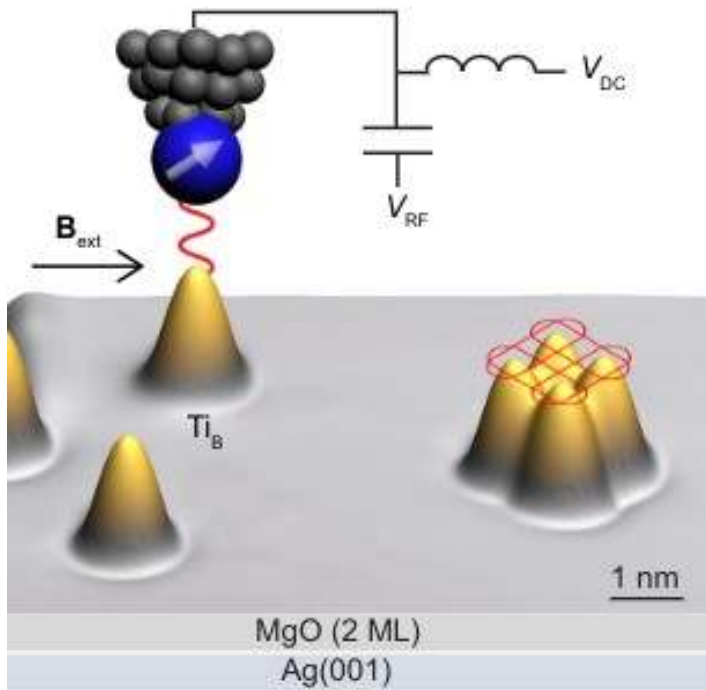
2D gaped bulk
0D fractional edge modes

Nature Nanotechnology (2024)
10.1038/s41565-024-01775-2

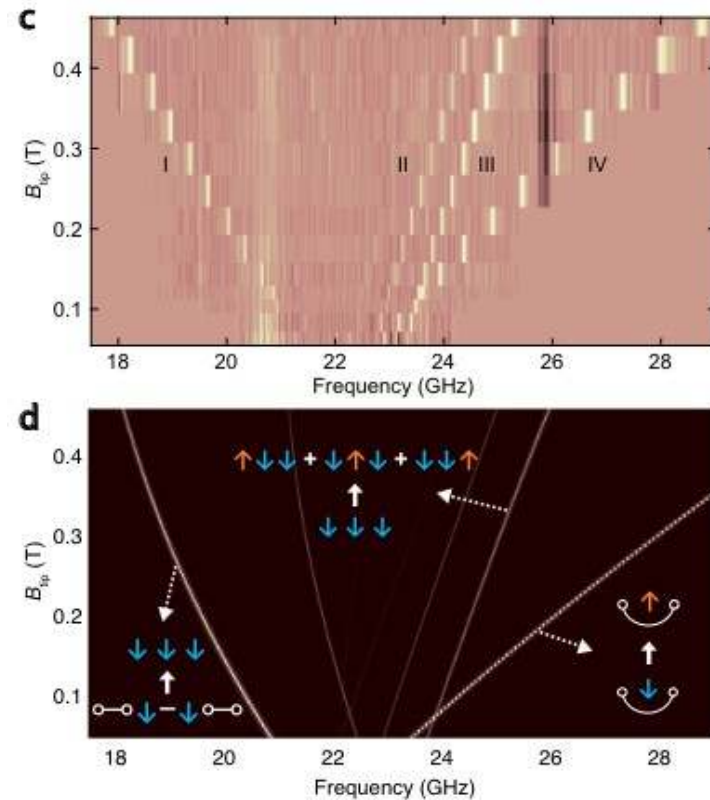
Artificial spin models with Ti@MgO

Ti@MgO

(2x2 lattice)

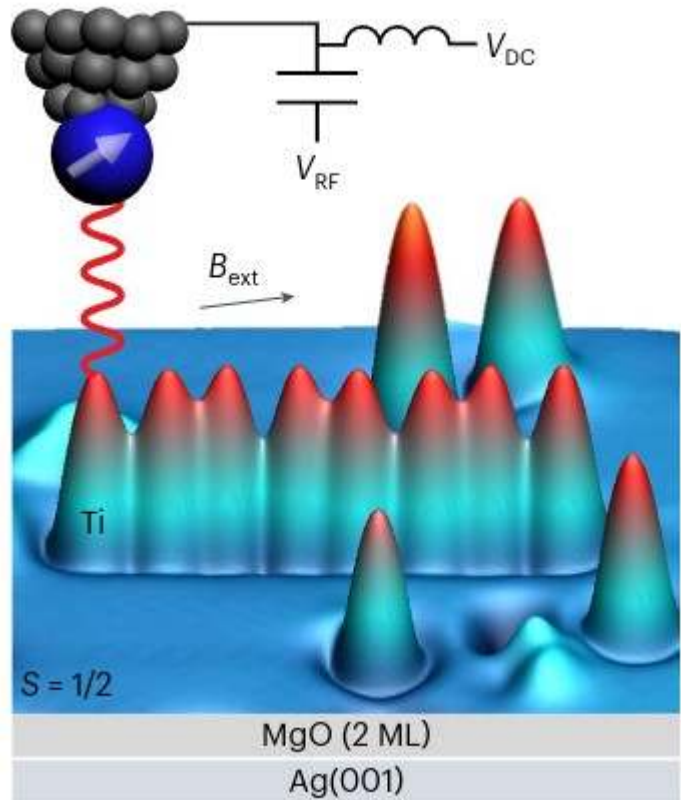


Nature Communications 12, 993 (2021)

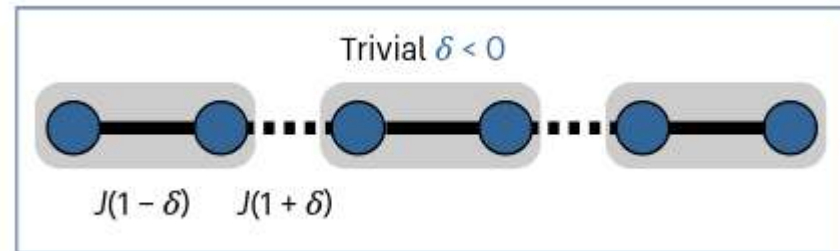
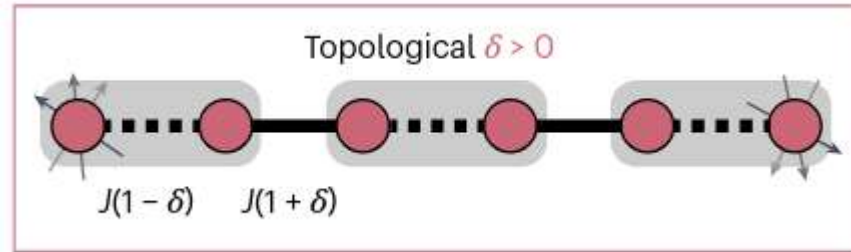


Can we create new states of matter?

First order topological quantum magnets



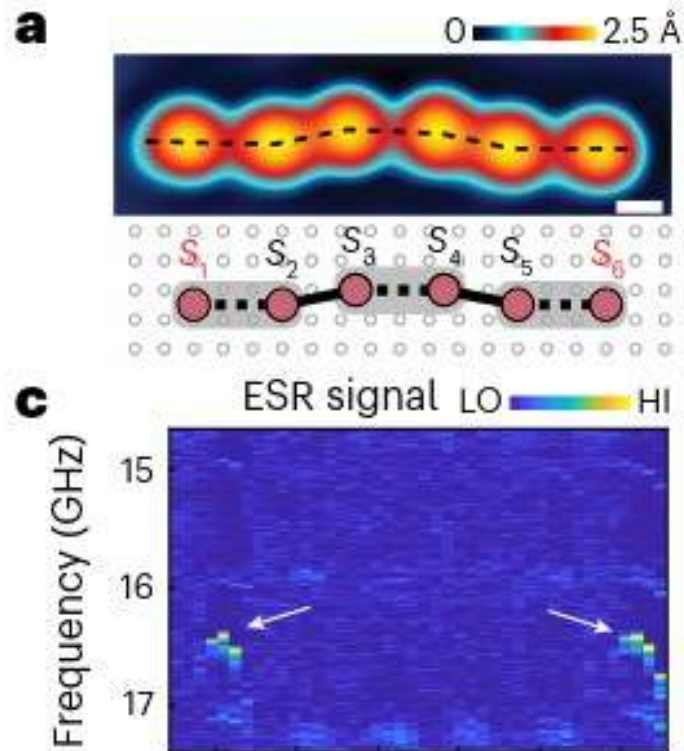
Two possible configurations



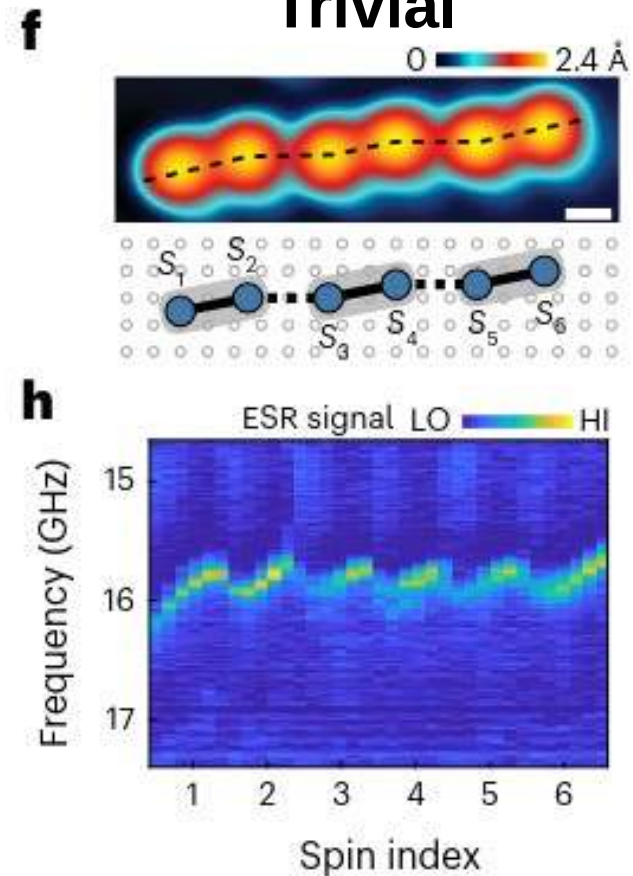
Nature Nanotechnology (2024)
10.1038/s41565-024-01775-2

First order topological quantum magnets

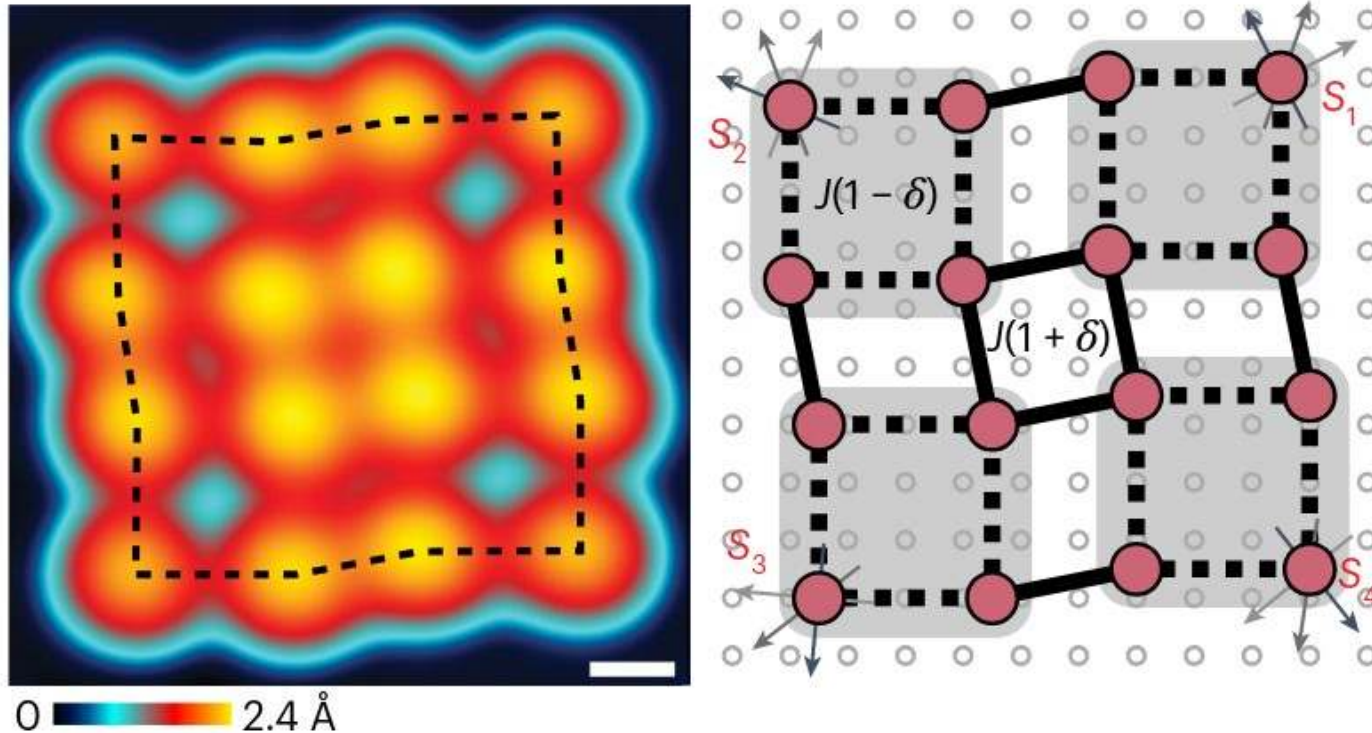
Topological



Trivial

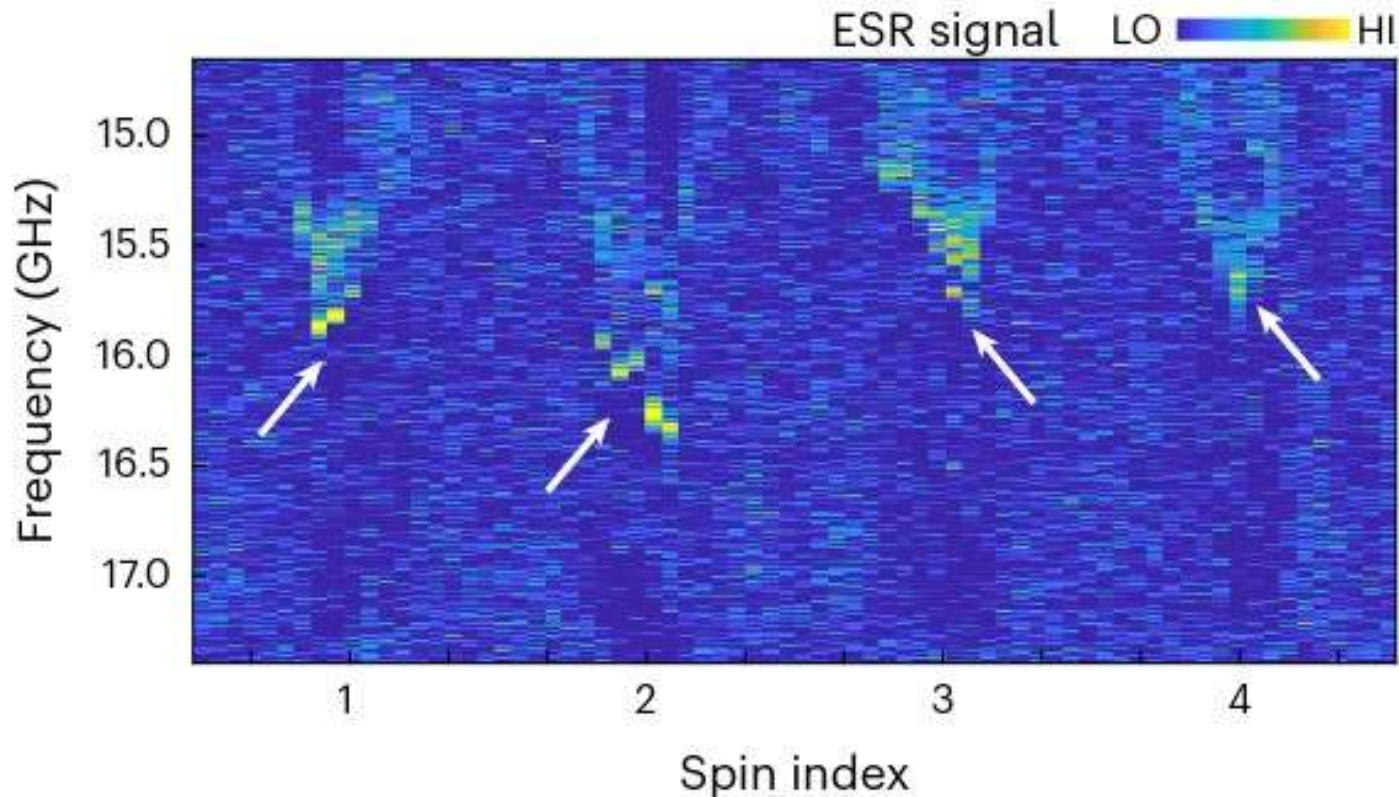


A higher order topological quantum magnet



The higher order topological quantum magnet shows topological corner modes

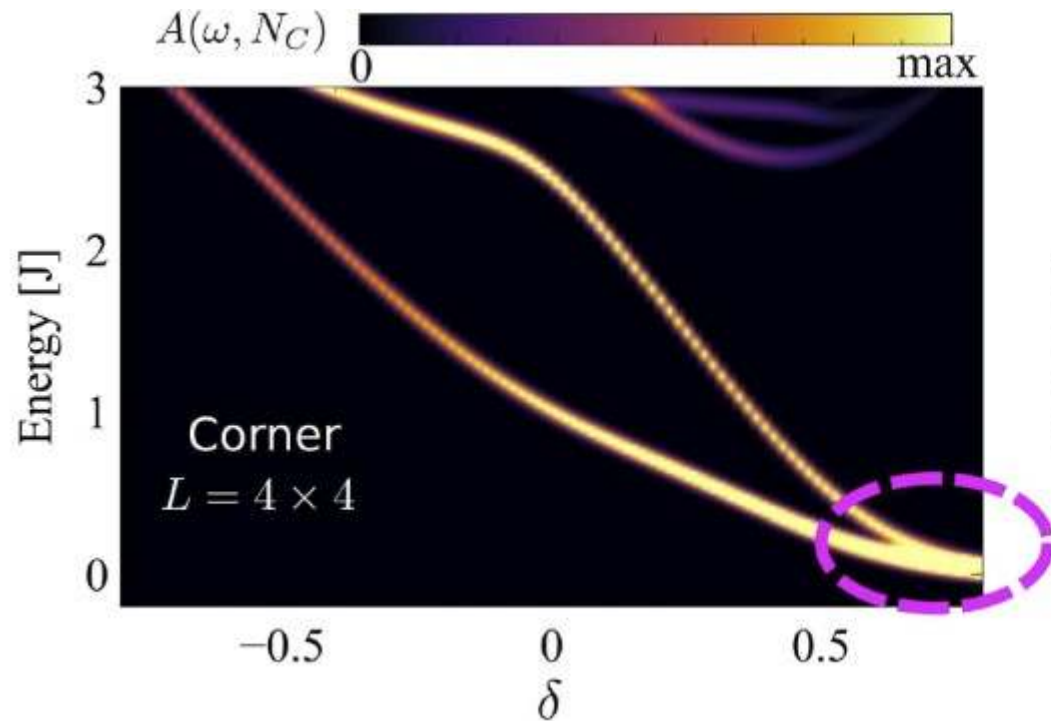
A higher order topological quantum magnet



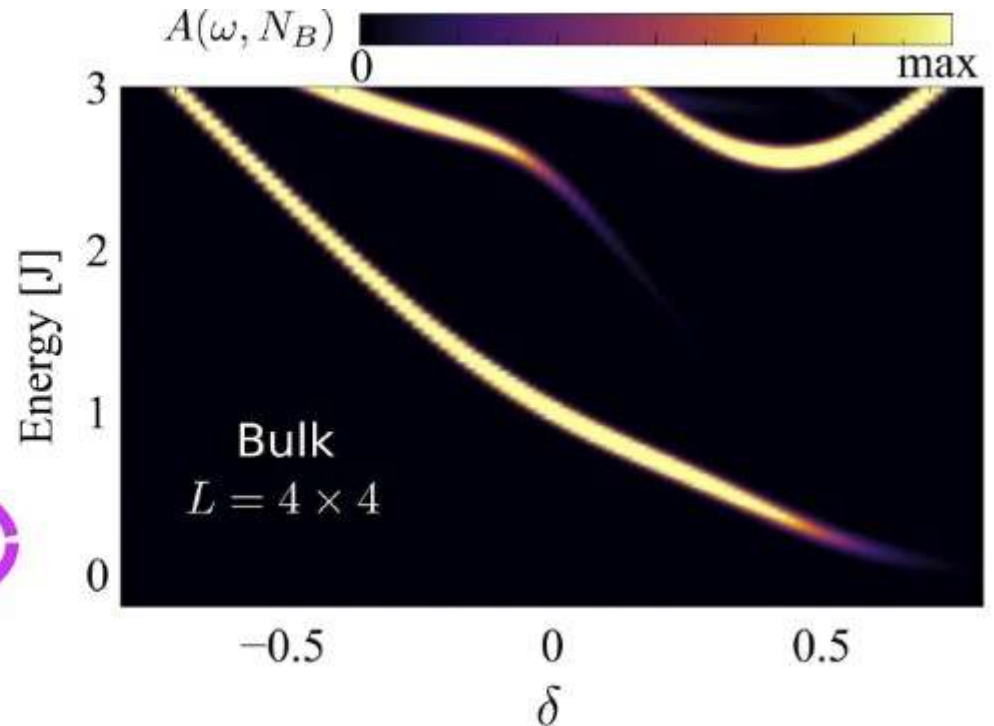
Topological corner modes are measured coexisting with a bulk spectral gap

A higher order topological quantum magnet

Corner spin excitations

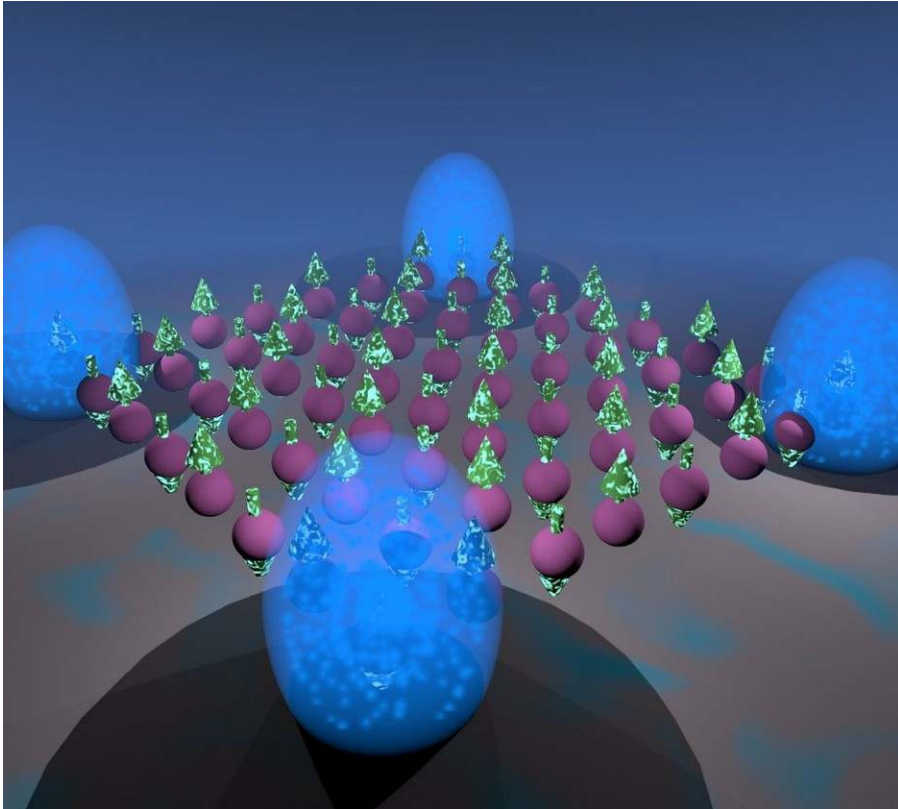


Bulk spin excitations



The tetramerization of the lattice creates topological corner spin excitations

The many-body phase diagram of a higher order topological quantum magnet

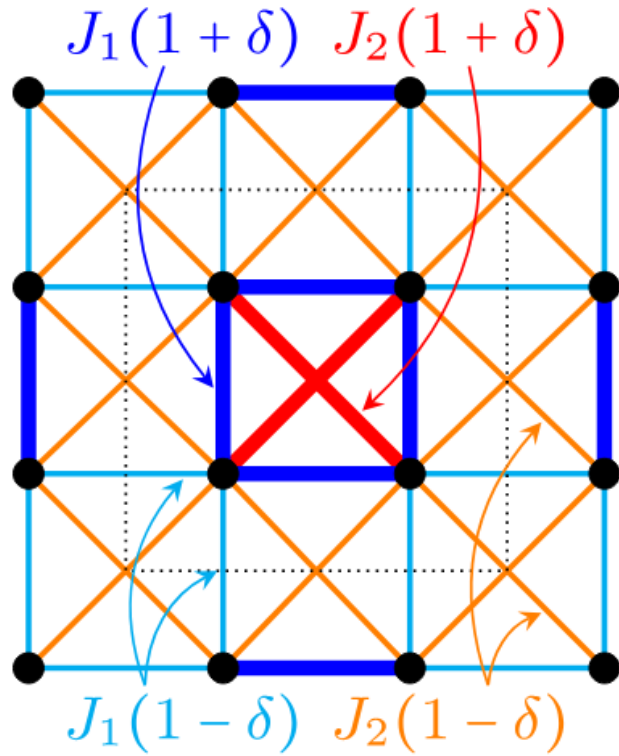


Pascal Vecsei

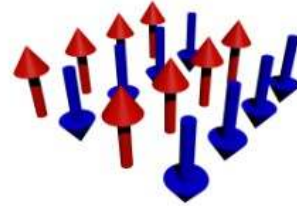


arXiv:2408.16453 (2024)

The model of a frustrated topological quantum magnet



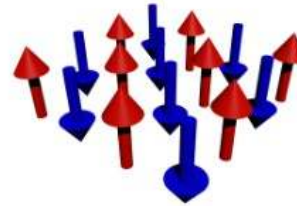
$$H = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$



Stripe
Antiferromagnet



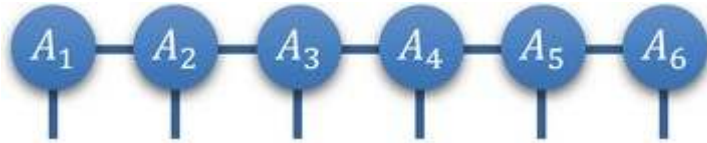
Topological
Quantum Magnet



Néel
Antiferromagnet

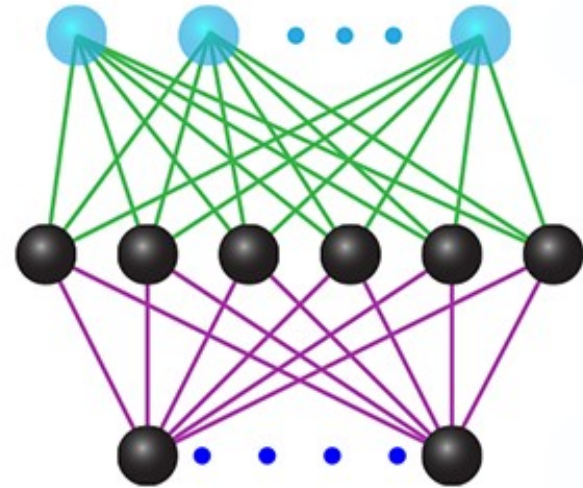
Solving frustrated quantum 2D models

Tensor-networks



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

Neural-network quantum states

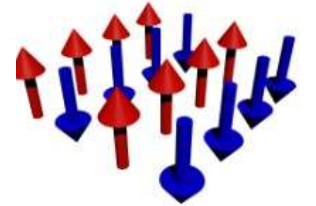
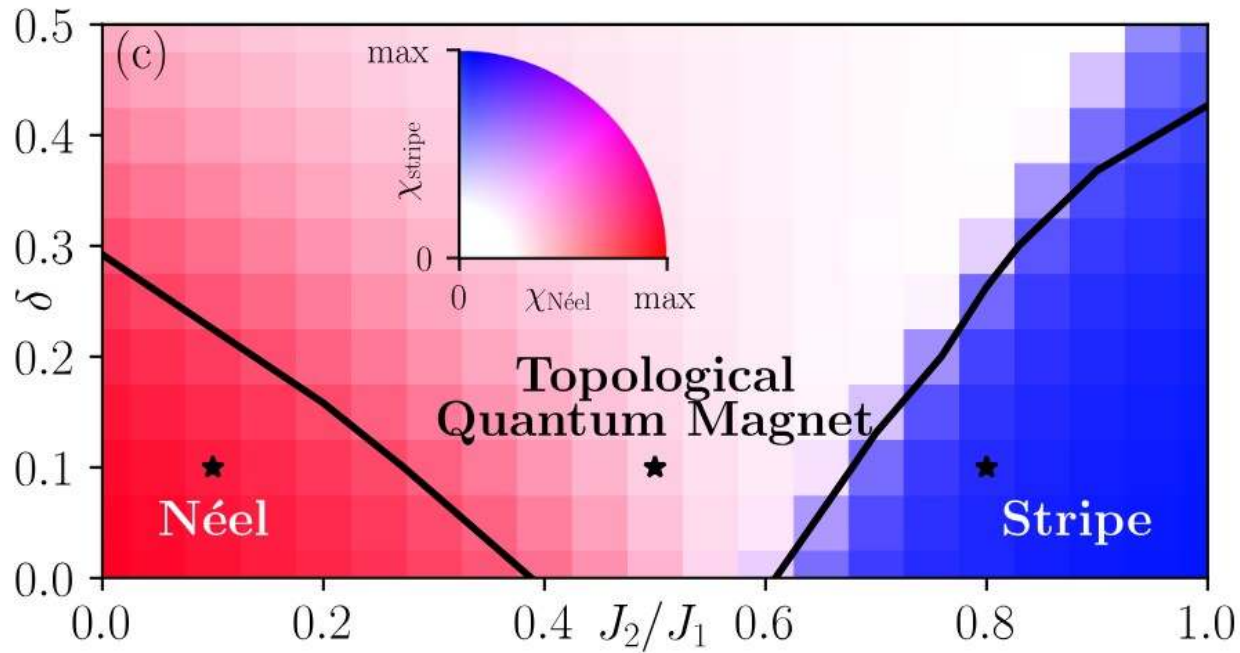


Science 355.6325 (2017): 602-606.

We use tensor networks and neural networks to solve frustrated many-body 2D systems with up to 100 quantum spins

The phase diagram of the higher order topological quantum magnet

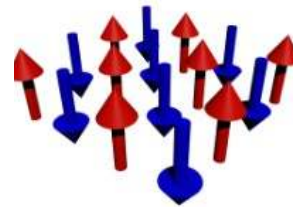
Phase diagram from susceptibilities



Stripe
Antiferromagnet



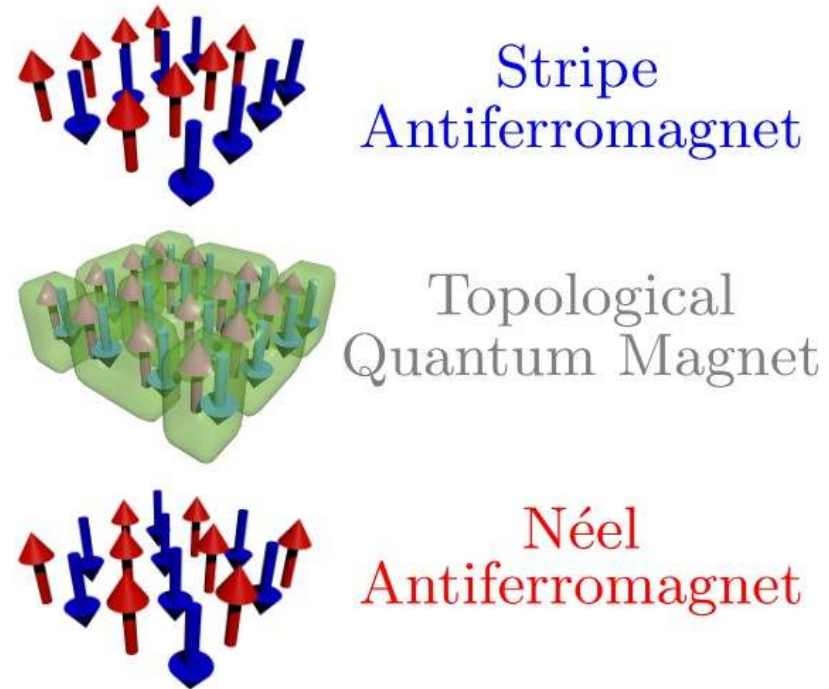
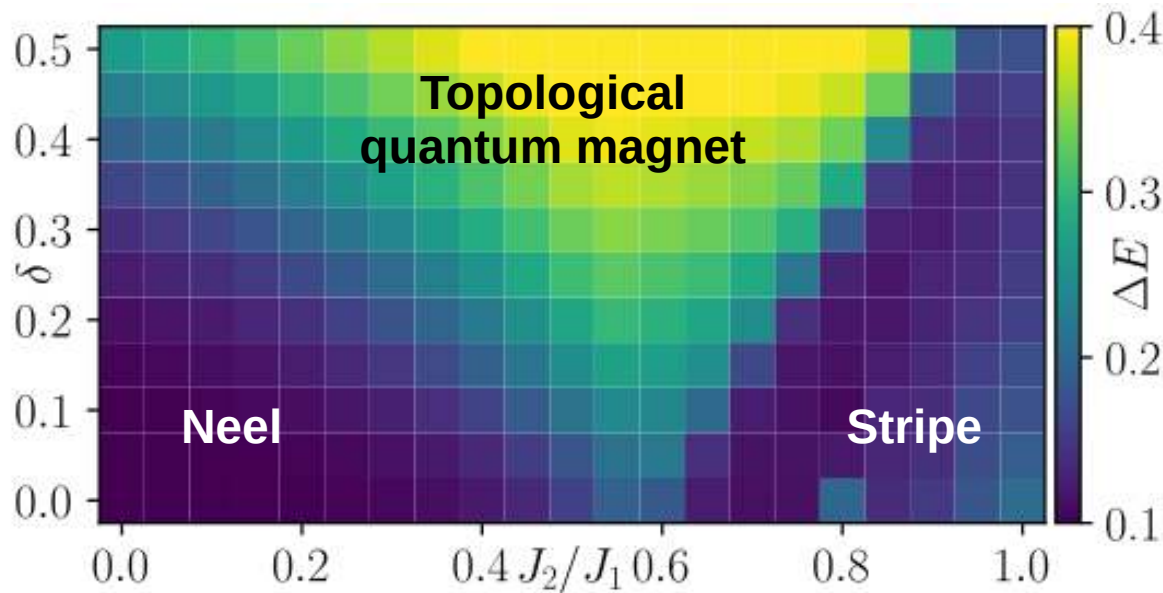
Topological
Quantum Magnet



Néel
Antiferromagnet

The phase diagram of the higher order topological quantum magnet

Phase diagram from many-body gaps



Stripe and Neel phase show gapless magnons, whereas the topological quantum magnet is gaped

The parton representation of a quantum magnet

Heisenberg model

$$H = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

Quantum disordered
ground state

Parton spinon
transformation

$$S_n^\alpha = \frac{1}{2} \sum_{s,s'} \sigma_\alpha^{s,s'} f_{n,s}^\dagger f_{n,s'}$$

$$\sum_s f_{n,s}^\dagger f_{n,s} = \mathcal{I}$$

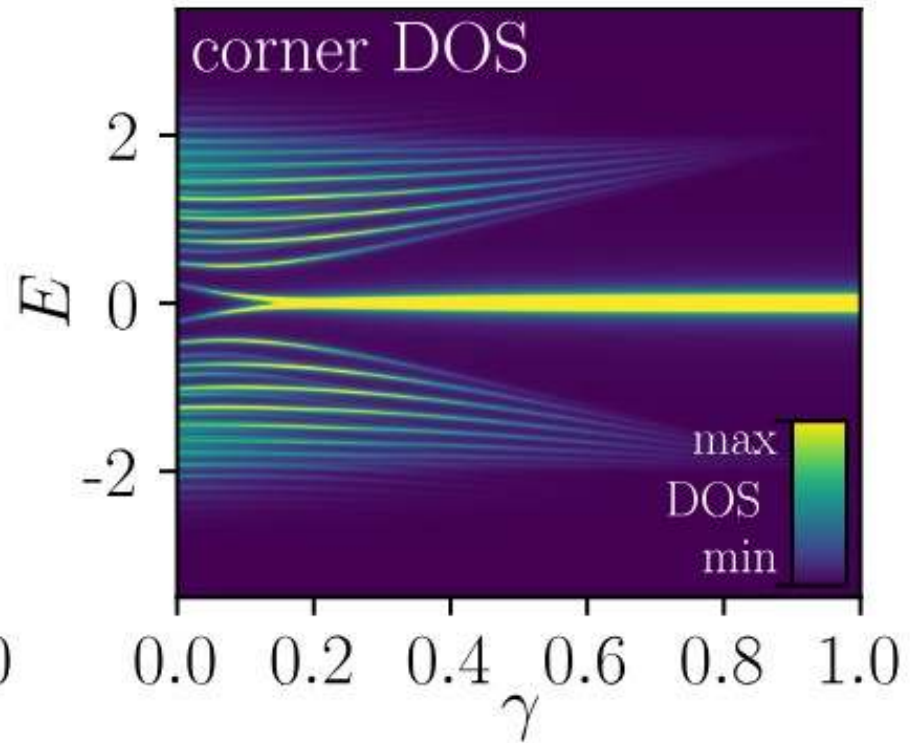
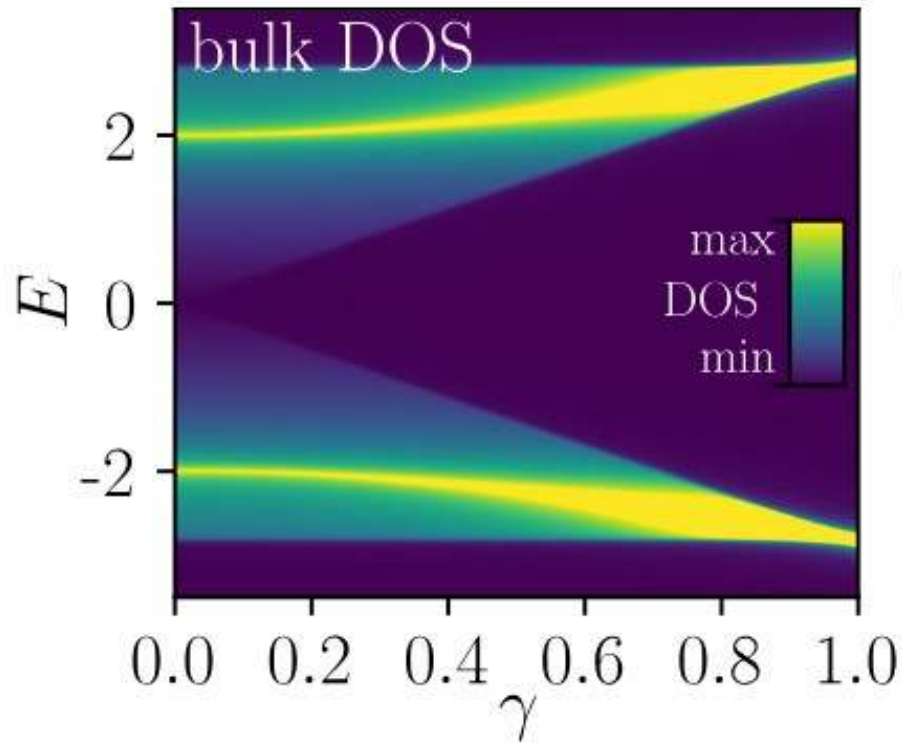
Spinon pi-flux model

$$\mathcal{H} = \sum_{ij} \Gamma_{ij} f_{i,s}^\dagger f_{j,s},$$

$$\prod_{ij} \text{sign}(\Gamma_{ij}) = -1$$

The topological nature of the ground state can be rationalized from parton replacement giving rise to a topological spinon model

Topological gap and gapless modes in the spinon representation



Gapless corner modes emerge, coexisting with the topological bulk gap

Open-source software for
artificial quantum materials

Open-source software for many-body quantum magnets

Python library for tensor-network kernel polynomial algorithms for spins, fermions, parafermions, with static solvers for Hermitian and non-Hermitian modes

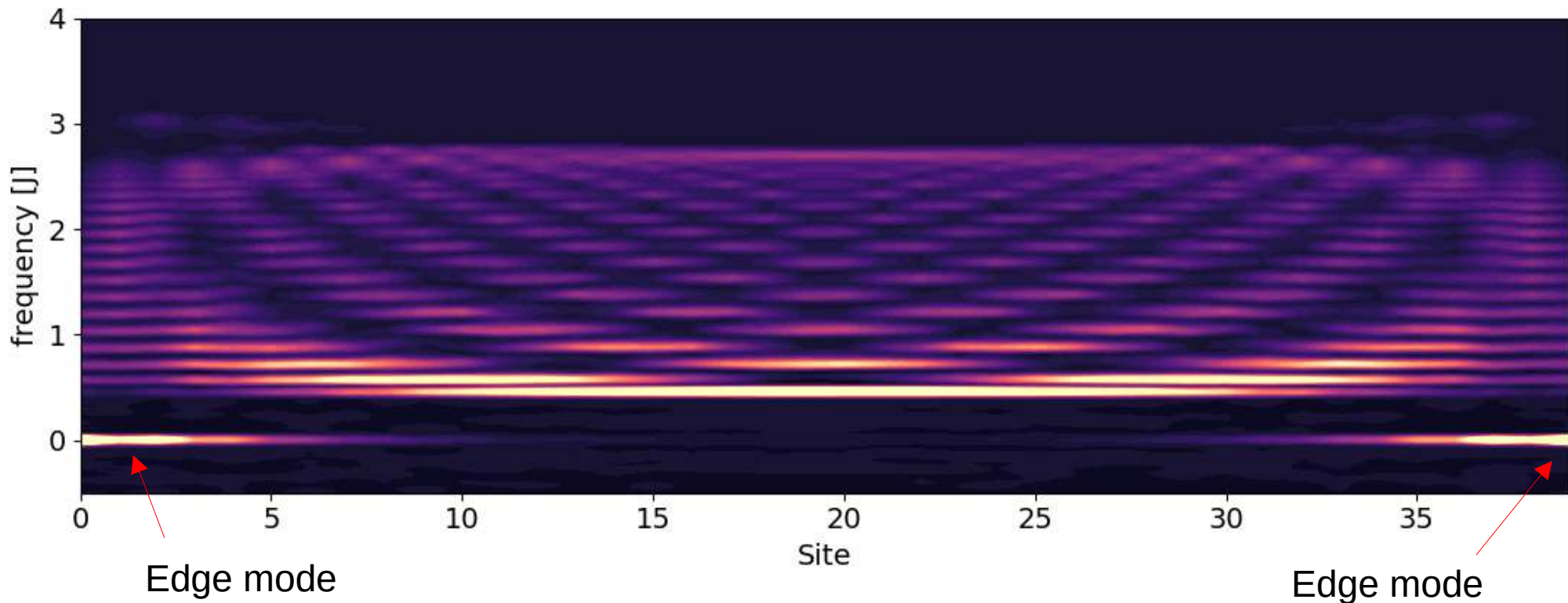
```
from dmrgpy import spinchain
spins = ["S=1" for i in range(40)] # S=1 chain
sc = spinchain.Spin_Chain(spins) # create spin chain object
h = 0 # initialize Hamiltonian
for i in range(len(spins)-1):
    h = h + sc.Sx[i]*sc.Sx[i+1]
    h = h + sc.Sy[i]*sc.Sy[i+1]
    h = h + sc.Sz[i]*sc.Sz[i+1]
sc.set_hamiltonian(h)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

dmrgpy

<https://github.com/joselado/dmrgpy>

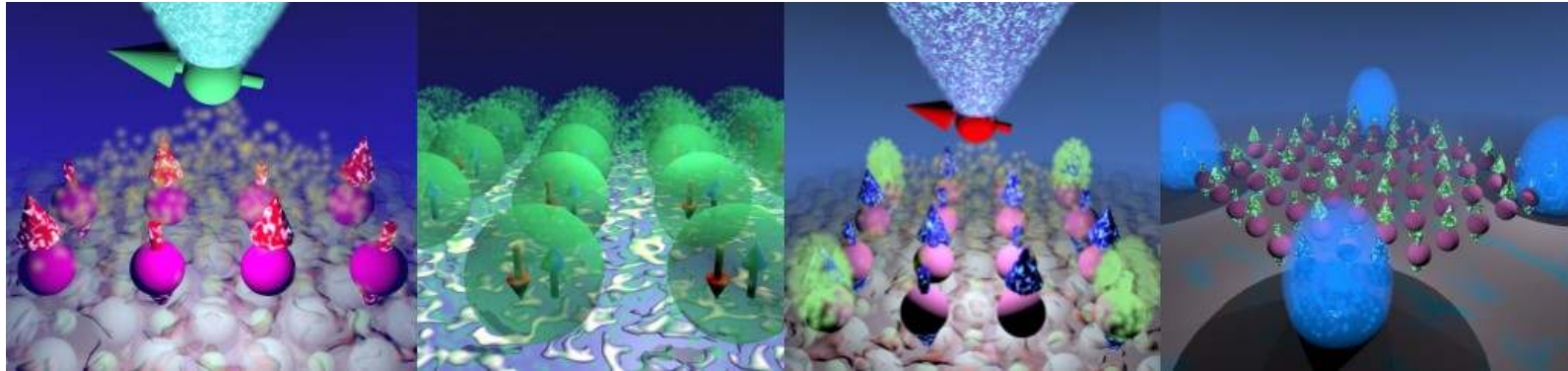
Open-source software for many-body quantum magnets

The spin spectral function of the $S=1$ Heisenberg model ($L=40$ sites)



Take home

Atomically engineered spin lattices allows us to create quantum matter with emergent quantum excitations



Phys. Rev. Lett. 131, 086701 (2023)

Phys. Rev. Applied 20, 024054 (2023)

Nature Nanotechnology (2024), 10.1038/s41565-024-01775-2

arXiv:2408.16453 (2024)

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Thank you