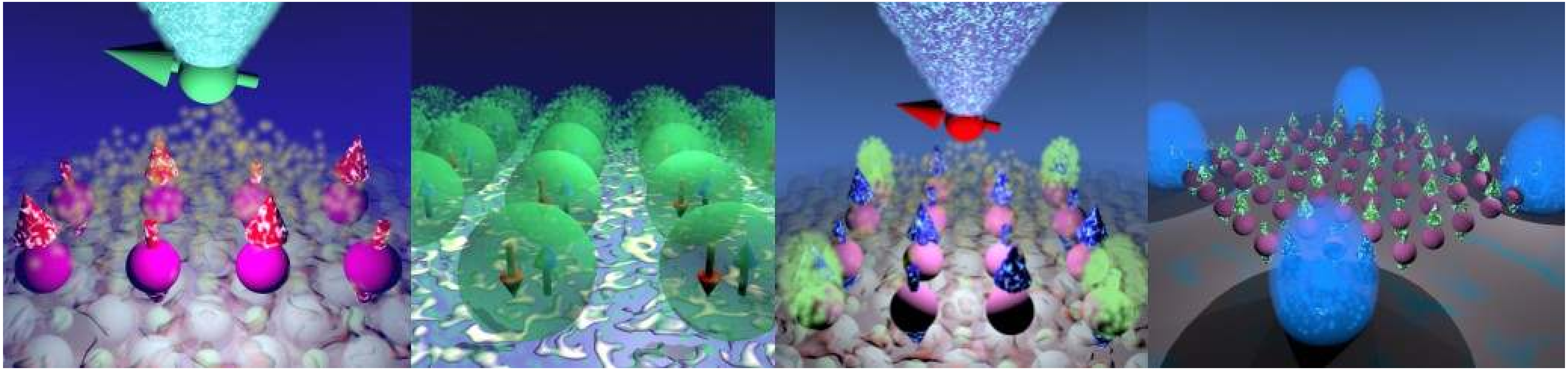
# Hamiltonian learning, triplons, and high-order topological order in engineered nanoscale quantum magnets

Jose Lado

*Department of Applied Physics, Aalto University, Finland*



*Phys. Rev. Appl 20, 024054 (2023)*

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

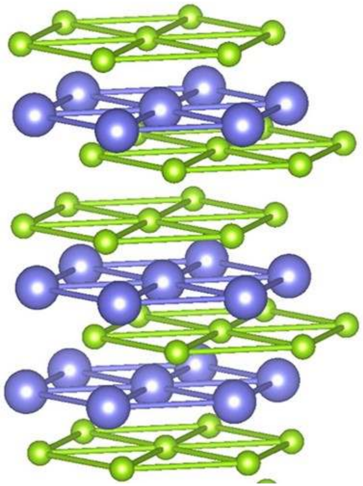
*Nature Nano (2024)*

*arXiv:2408.16453 (2024)*

Carbon-based nanostructures with engineered electronic and spin properties, CMD31, Portugal September 4$^{th}$ 2024

# Emergence in quantum materials

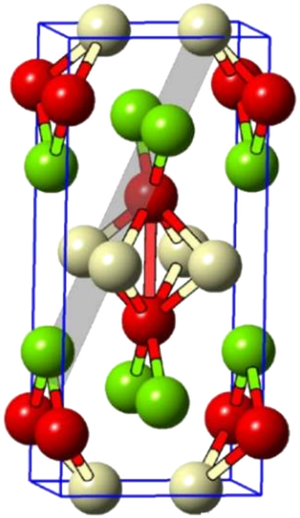
**Topological materials**



$Bi_2Se_3$

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

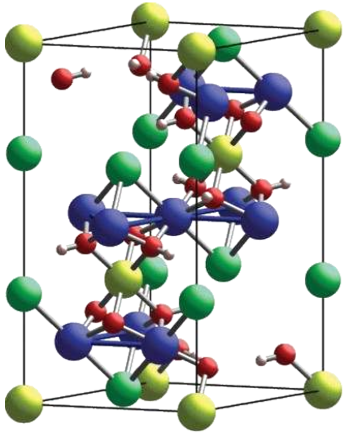
**Unconventional superconductors**



$UTe_2$

*Nature 579, 523–527 (2020)*

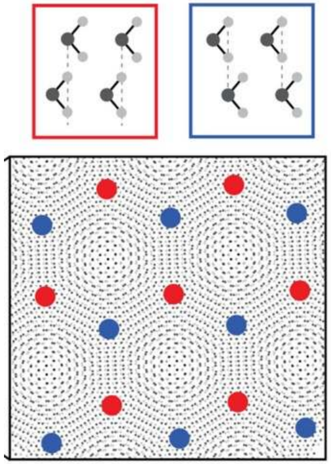
**Quantum spin liquids**



$ZnCu_3(OH)_6Cl_2$

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

**Fractional topological matter**

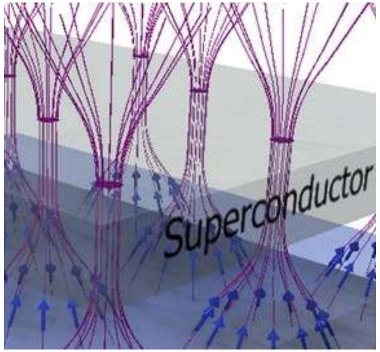


Twisted $MoTe_2$

*Nature (2023)*

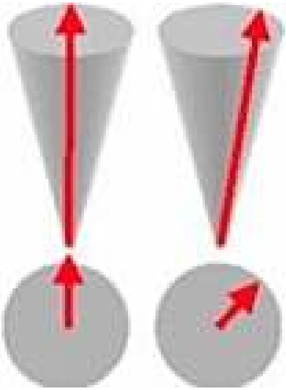
# Emergent excitations in quantum materials

Vortexes




***Superconductors***

Magnons

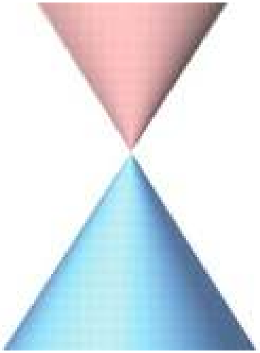


***Ordered magnets***

Skyrmions

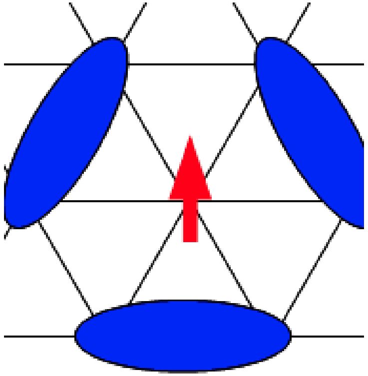
**Non-collinear magnets**

Dirac fermions



***Topological materials***

Spinons

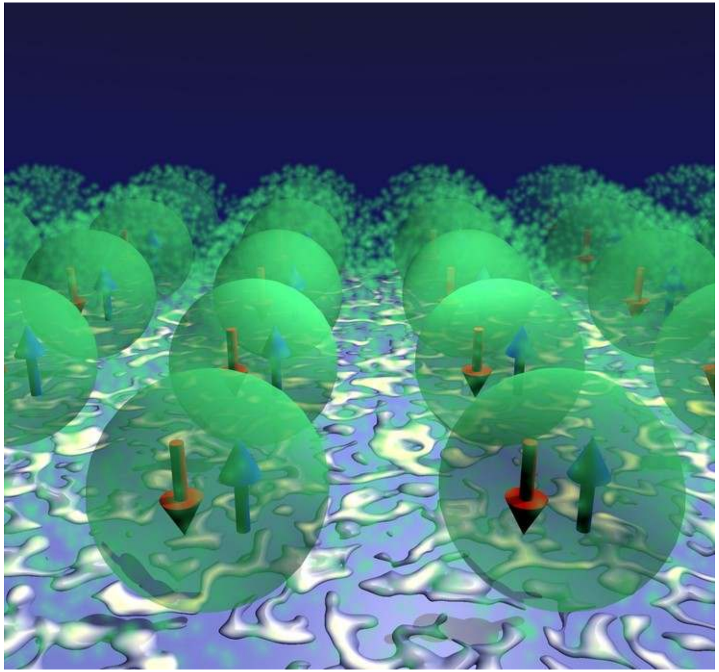


***Quantum spin liquids***

***The discovery of new quasiparticles opens new possibilities in quantum technologies***

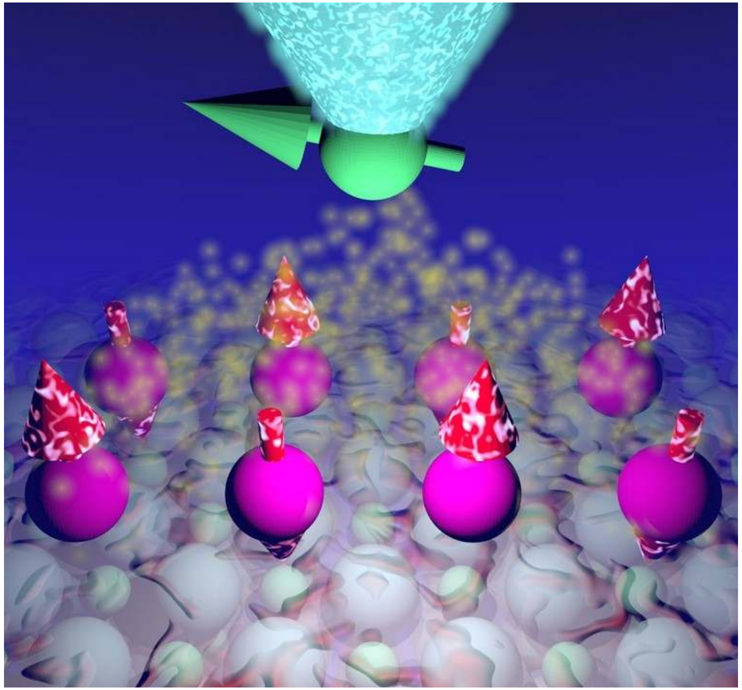
# Plan for today

**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

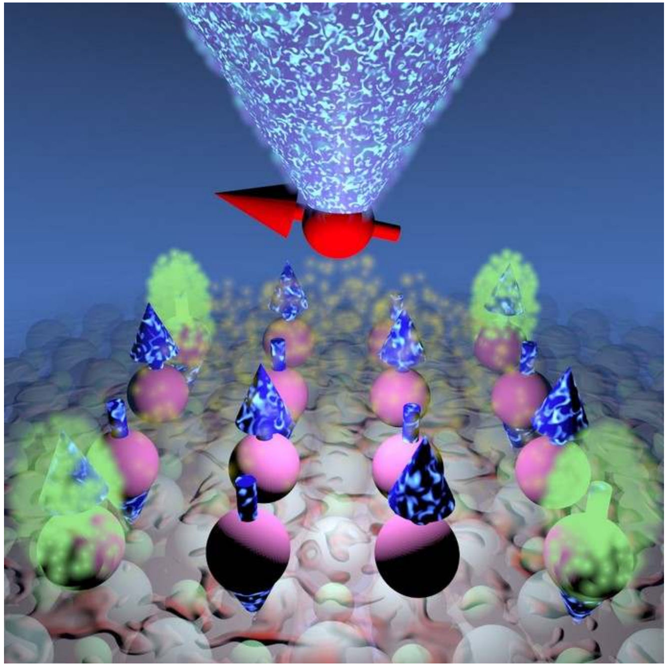
Guangze Chen

Adolfo Fumega

Phys. Rev. Applied 20, 024054 (2023)

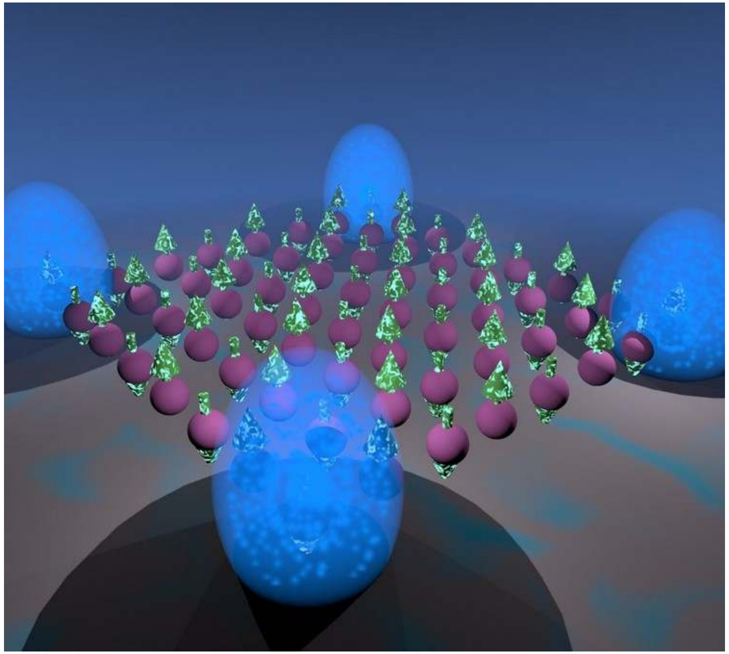
# Plan for today

**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

Jing Chen

Lili Jiang

Peng Fang

Hong-Jun Gao

Kai Yang

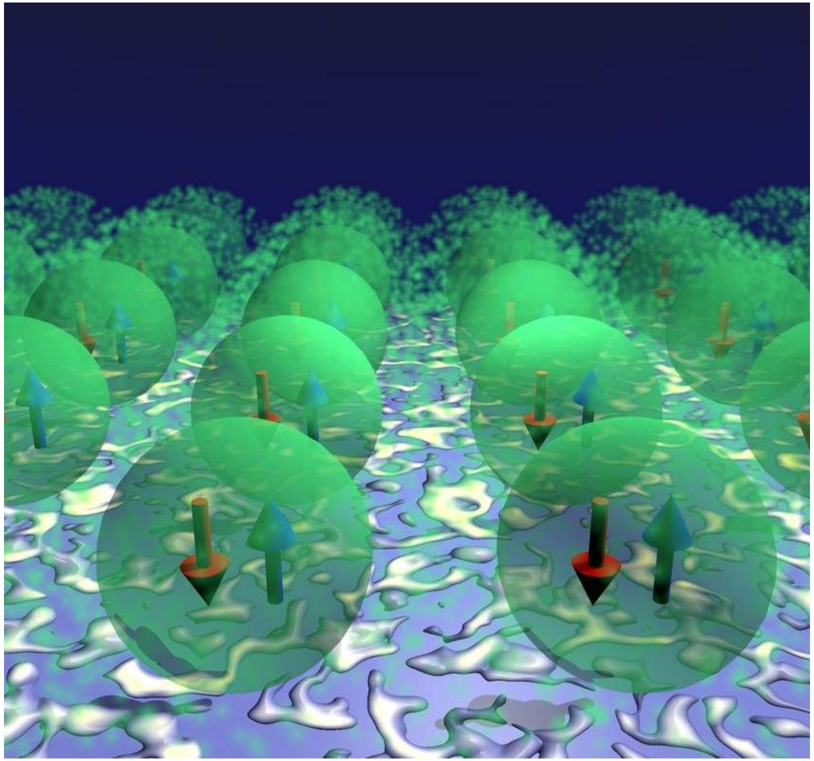
Nature Nanotechnology (2024), 10.1038/s41565-024-01775-2

**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)

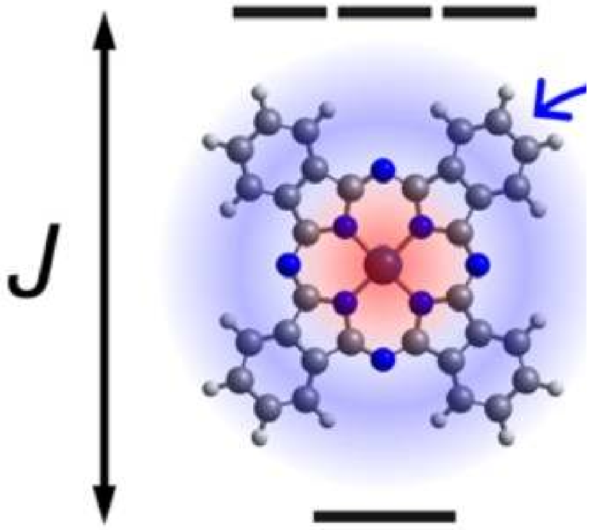
**Triplons in an atomic-scale quantum magnet**

Robert Drost

Shawulienu Kezilebieke

Peter Liljeroth

# Triplet excitations in a molecule




S = 1

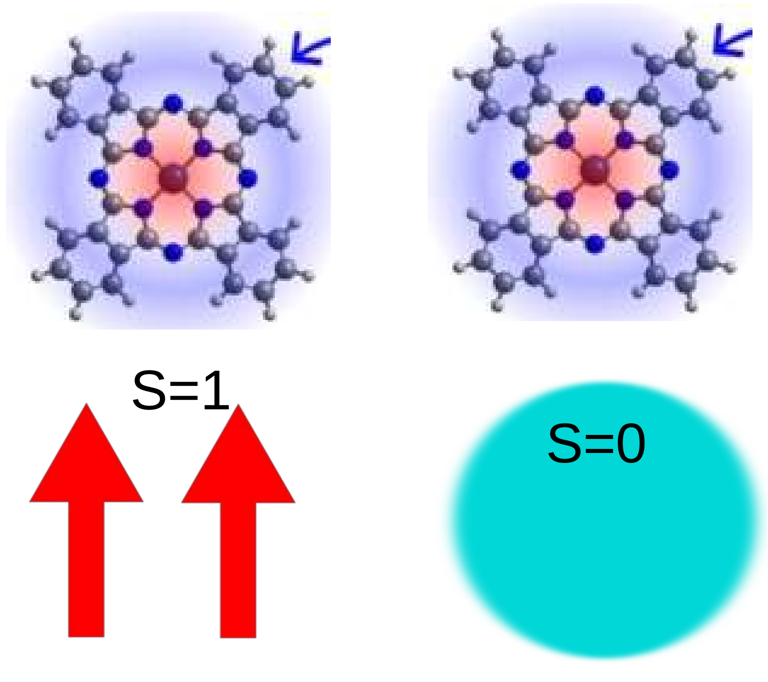
S = 0

Internal antiferromagnetic coupling

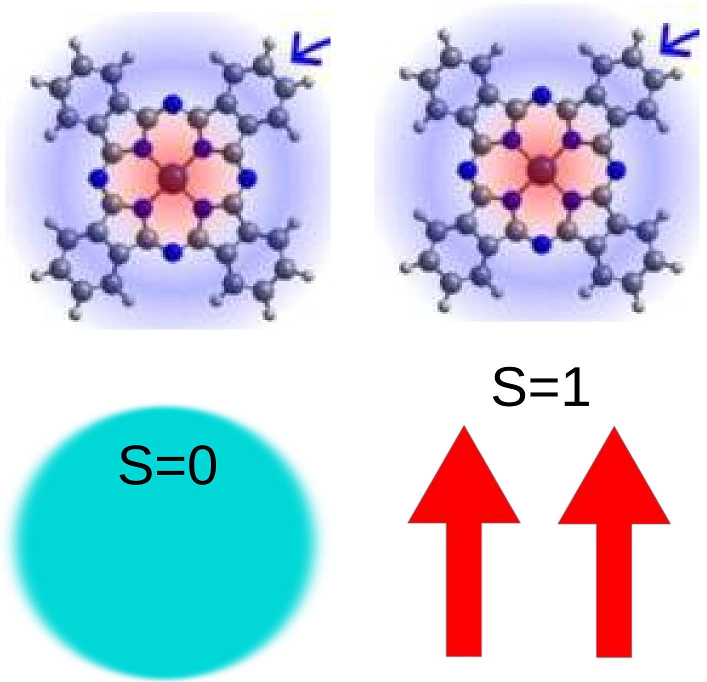
$$H = J\mathbf{S}\cdot\mathbf{K}$$

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

# Triplons in a dimer



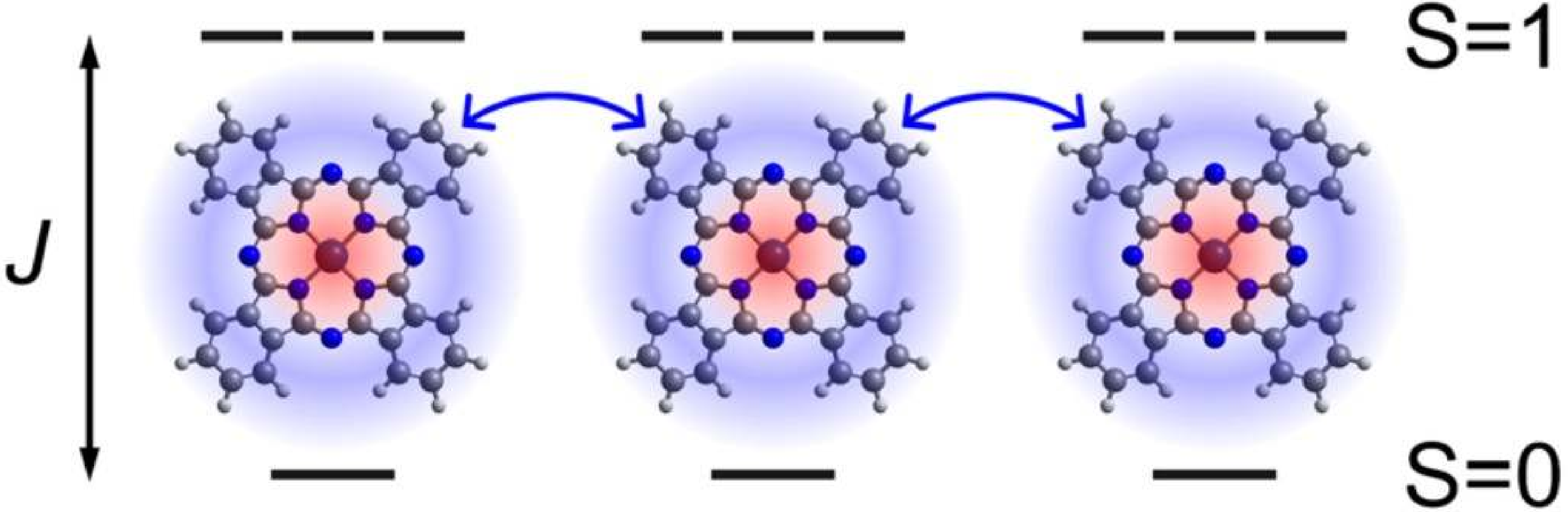

A triplet in the first molecule




Can jump to the second molecule

**Exchange coupling between molecules leads to propagating triplon excitations**

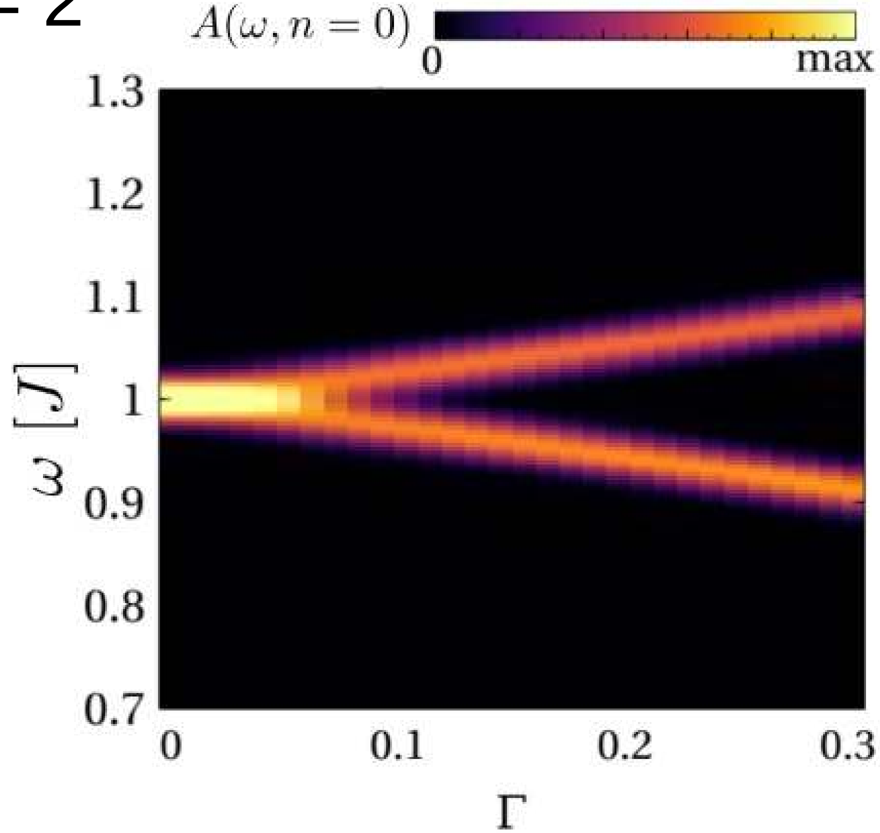
# A chain of triplons



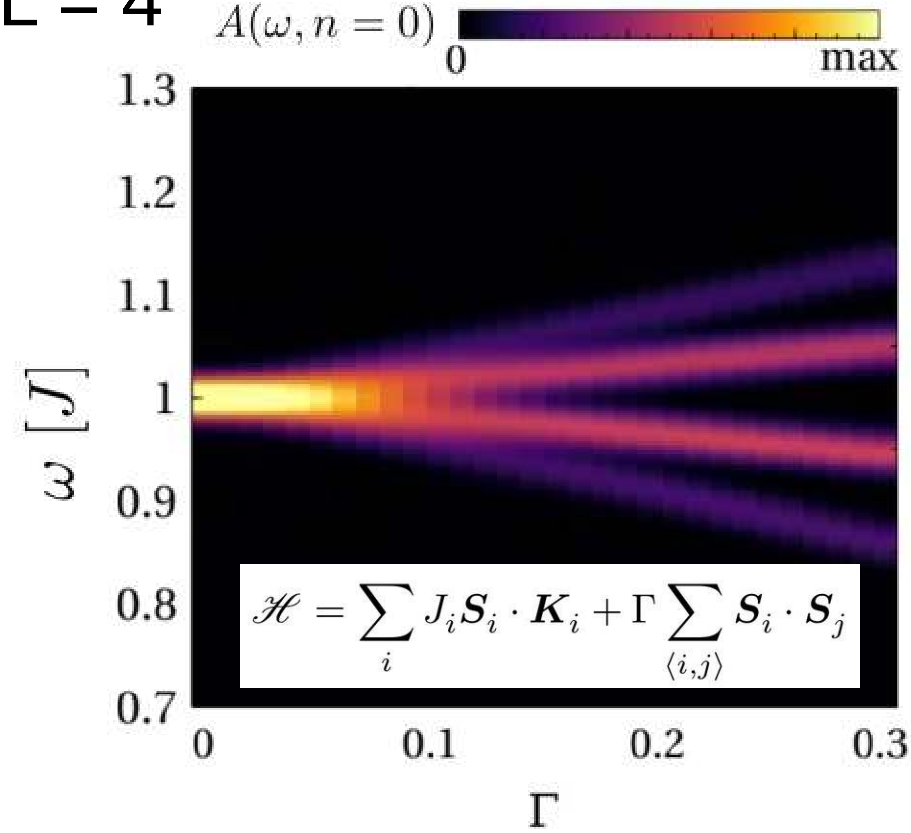

$$\mathscr{H} = \sum_i J_i \boldsymbol{S}_i \cdot \boldsymbol{K}_i + \Gamma \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

# Chains of triplons

L = 2

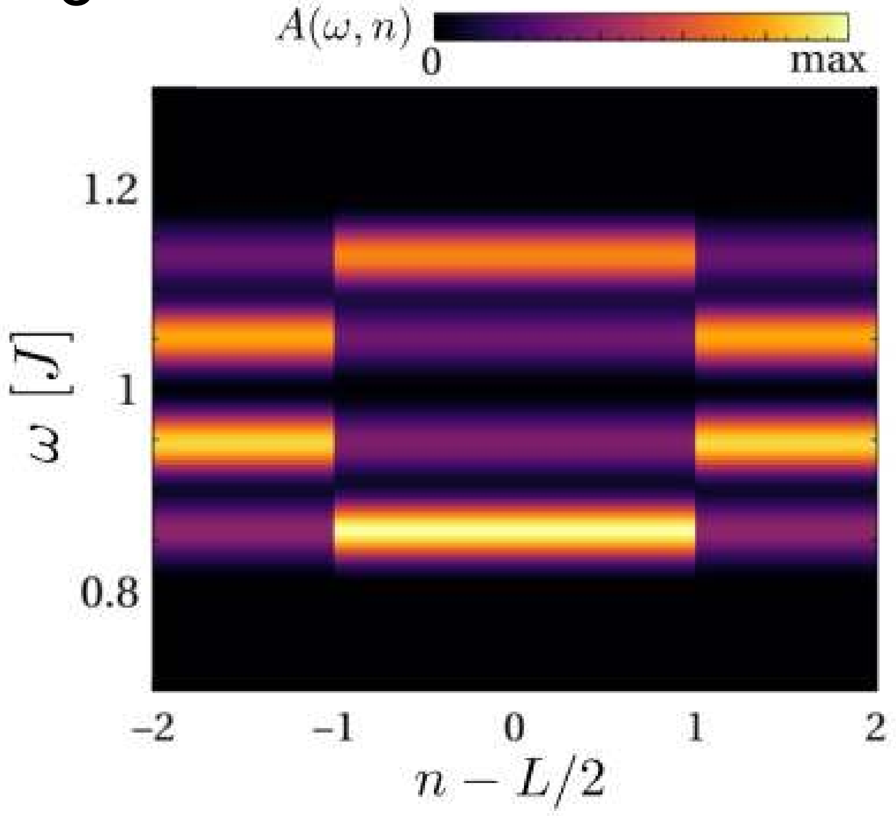



L = 4

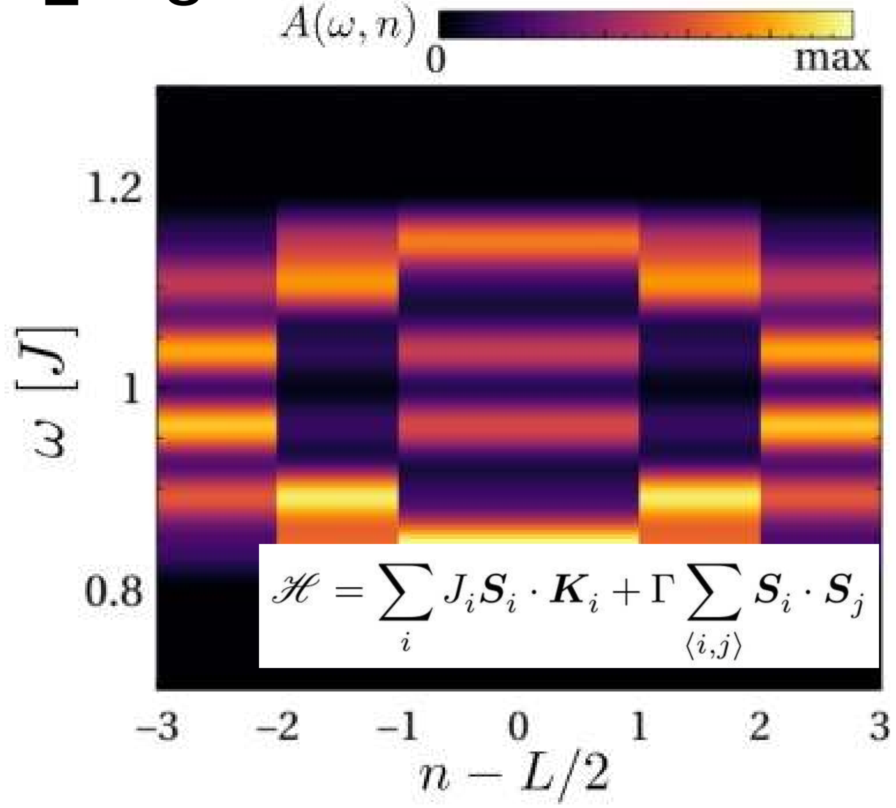


# Chains of triplons

L = 6



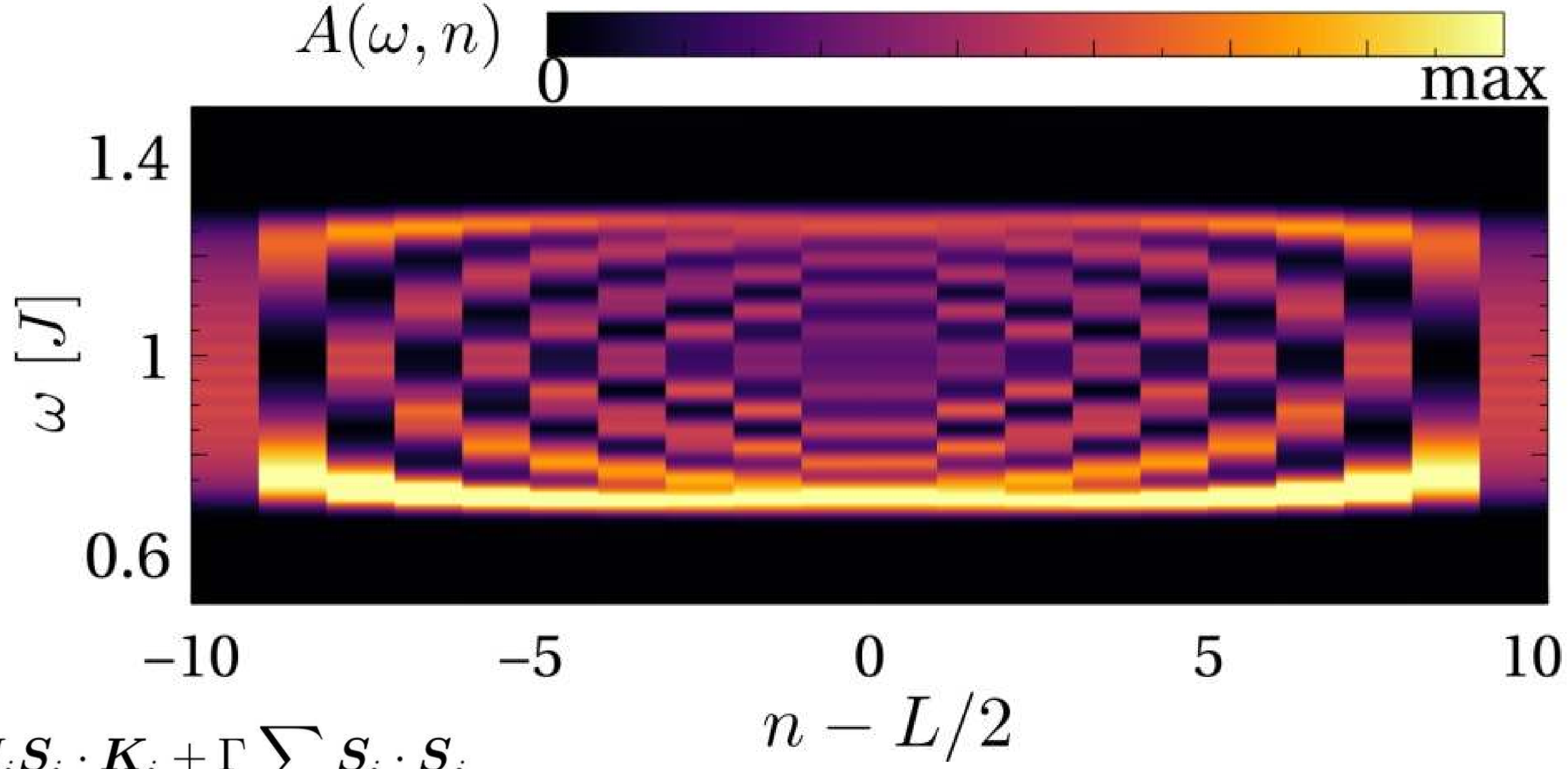

L = 8




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

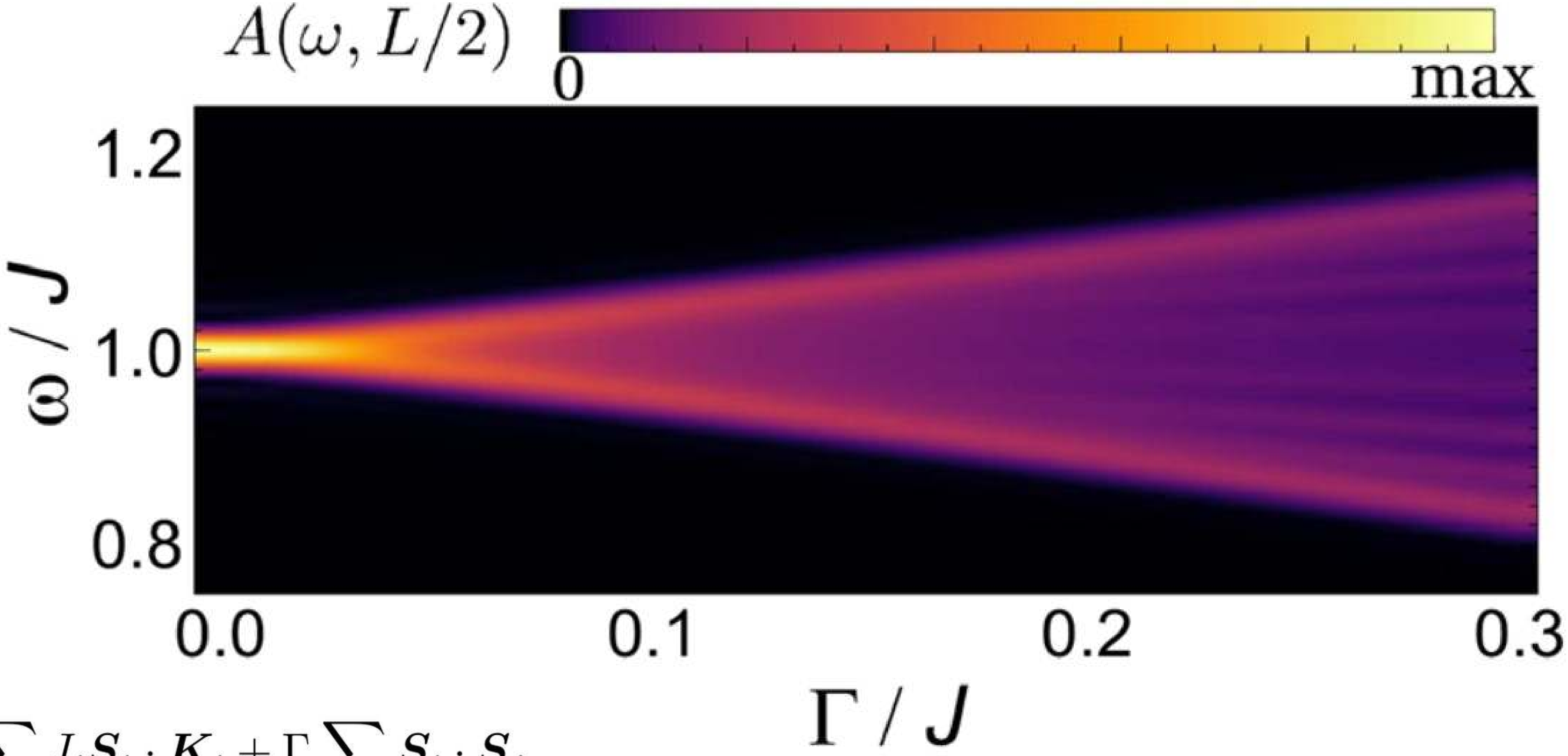
# Chains of triplons

L = 20




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

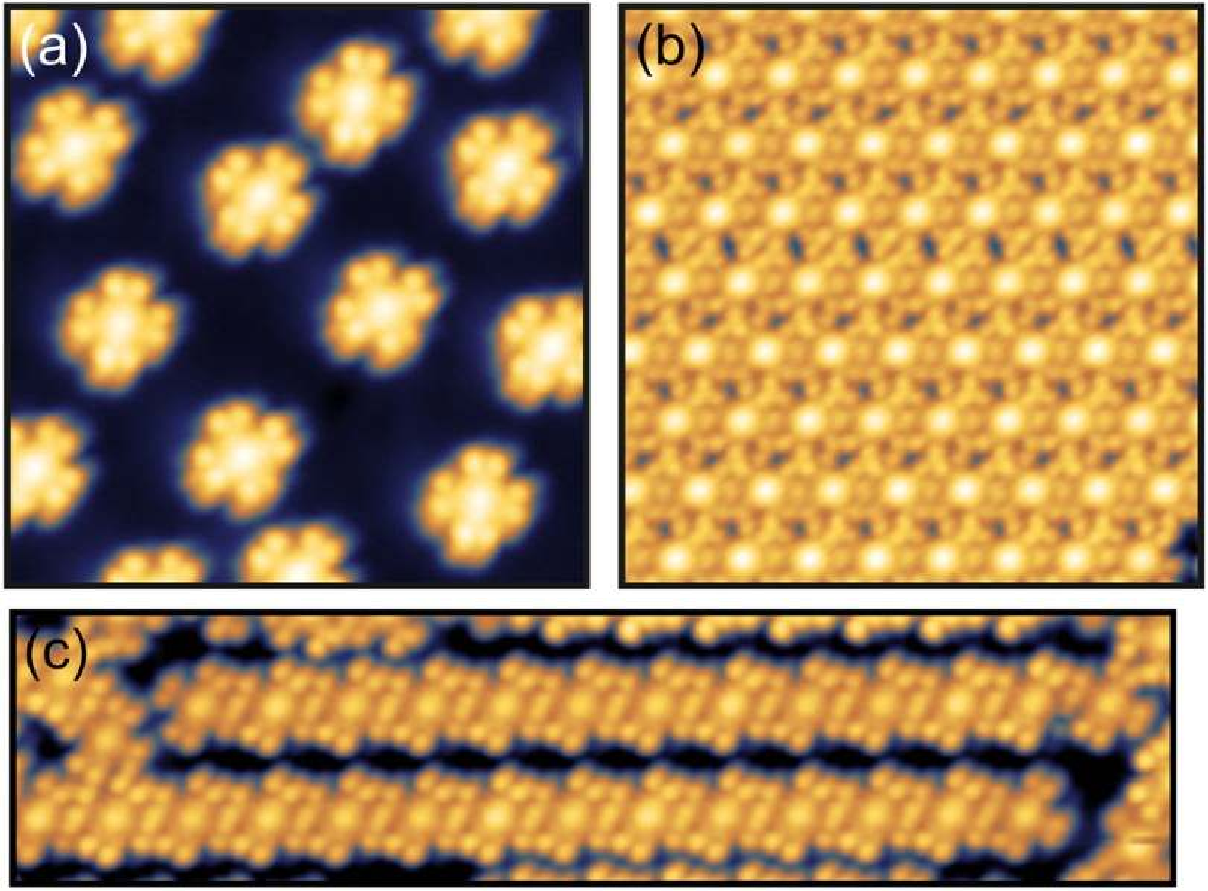
# Chains of triplons




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

# 0D, 1D and 2D arrays

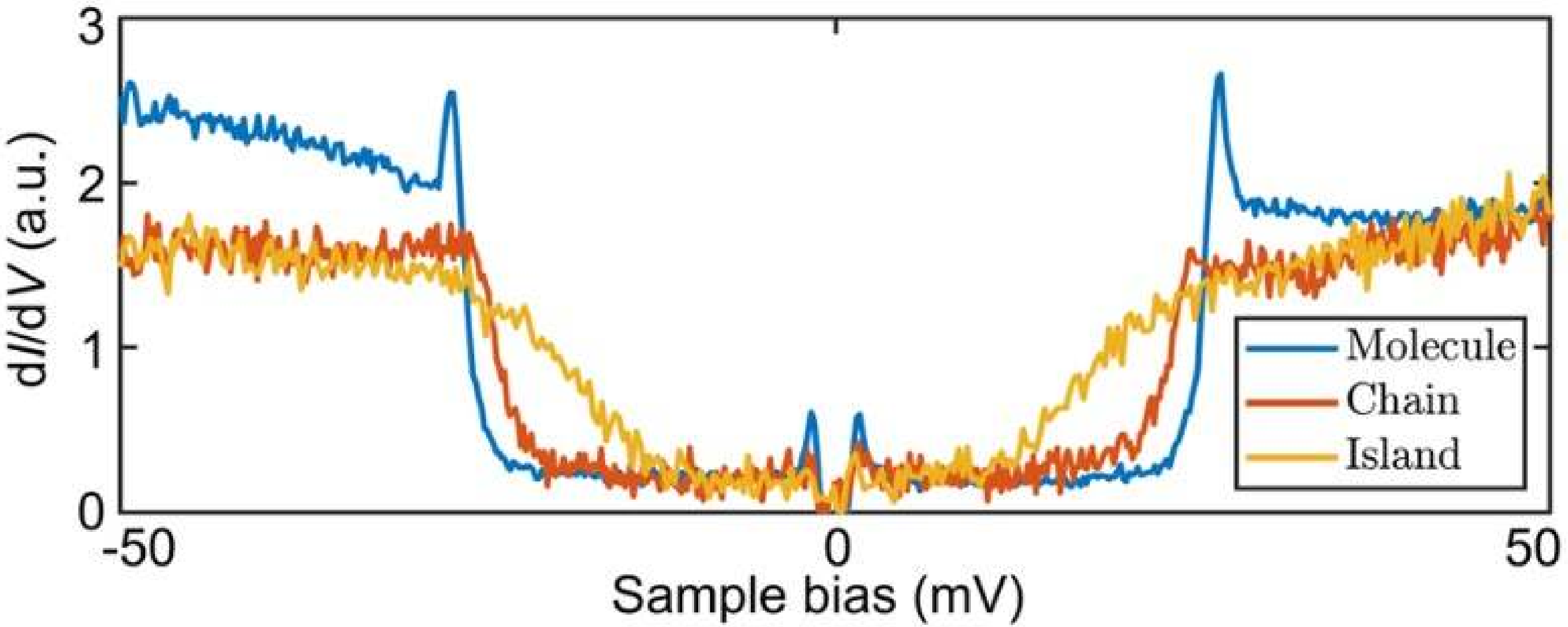
0D




2D

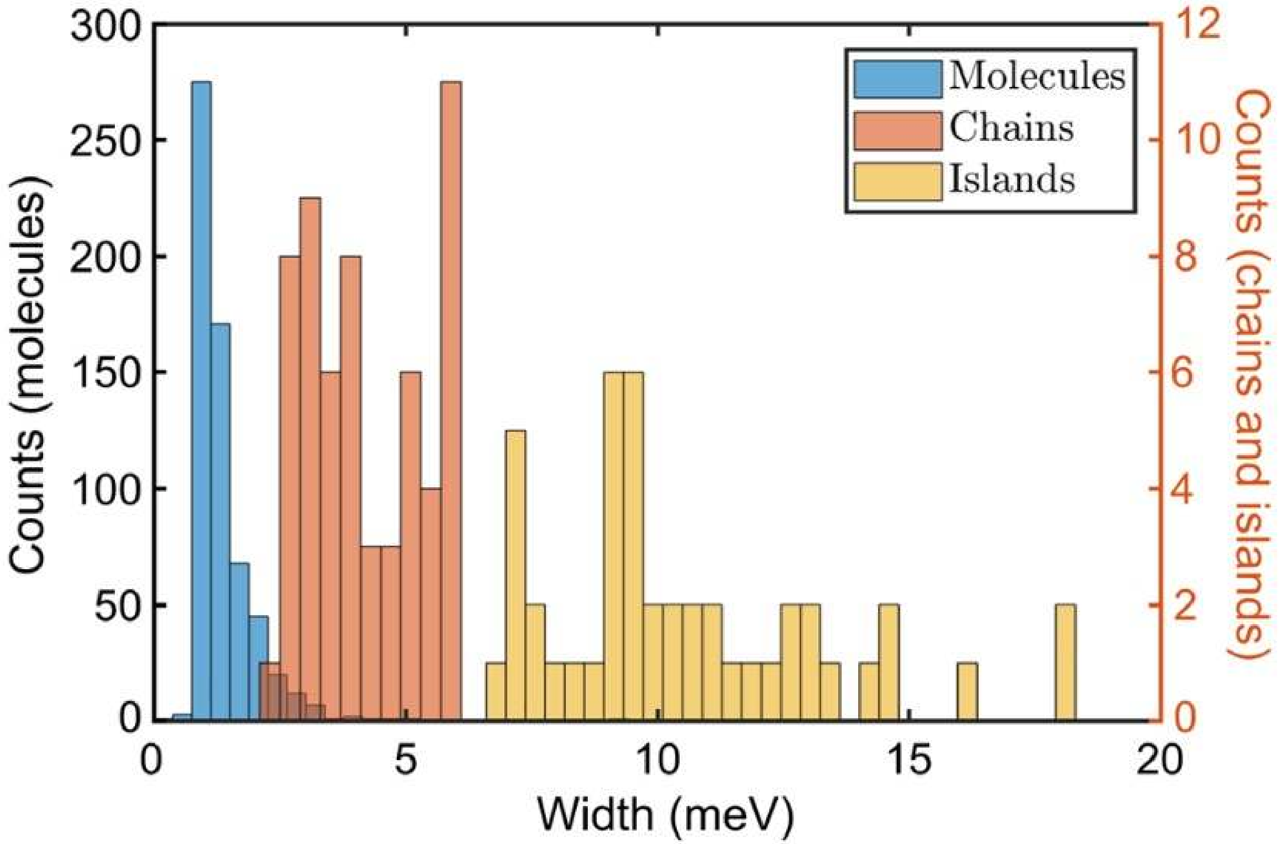
1D

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



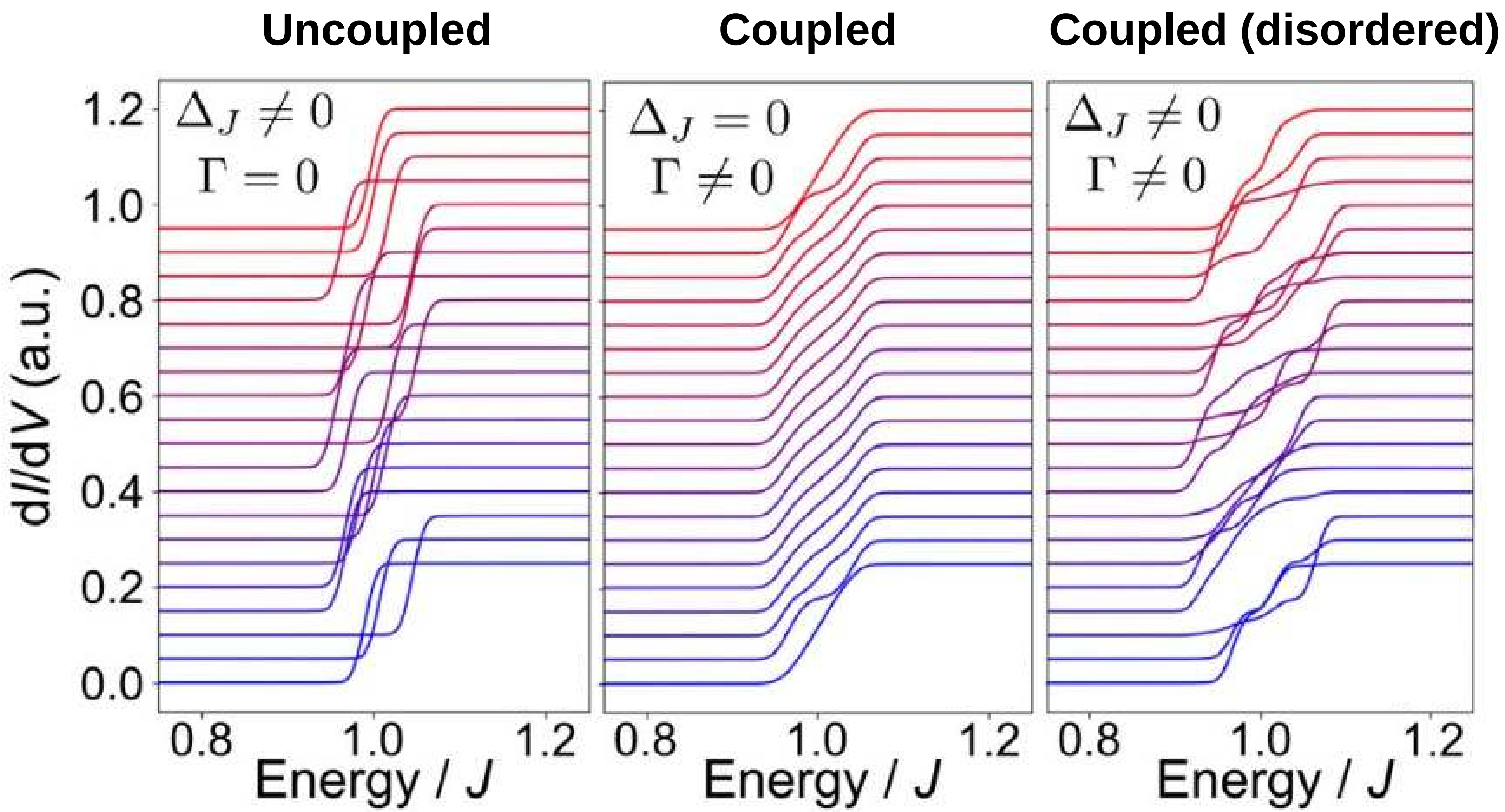

**The width of the step is bigger for islands than for molecules**

# Statistic of the inelastic steps

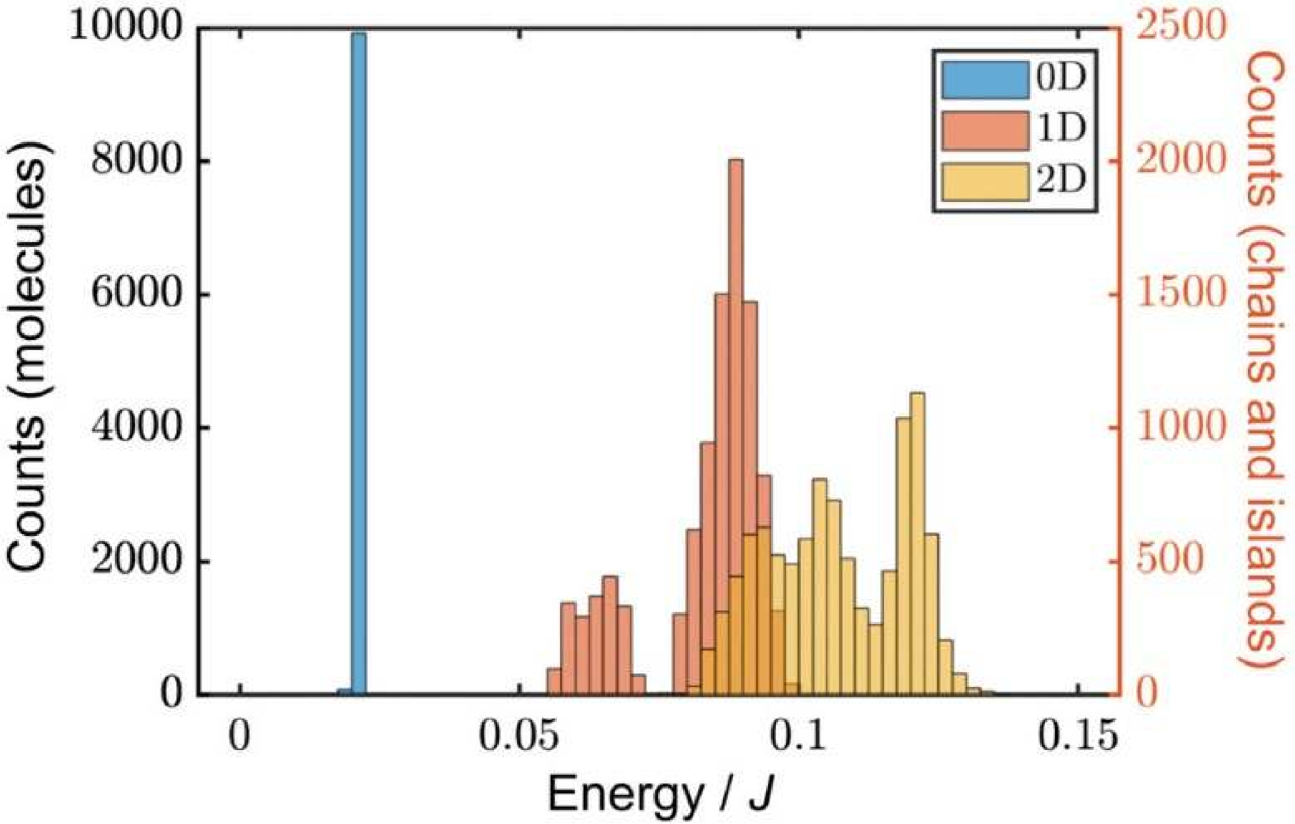



**2D arrays have the largest width of the spin excitation**

# Coupled and uncoupled inelastic excitation

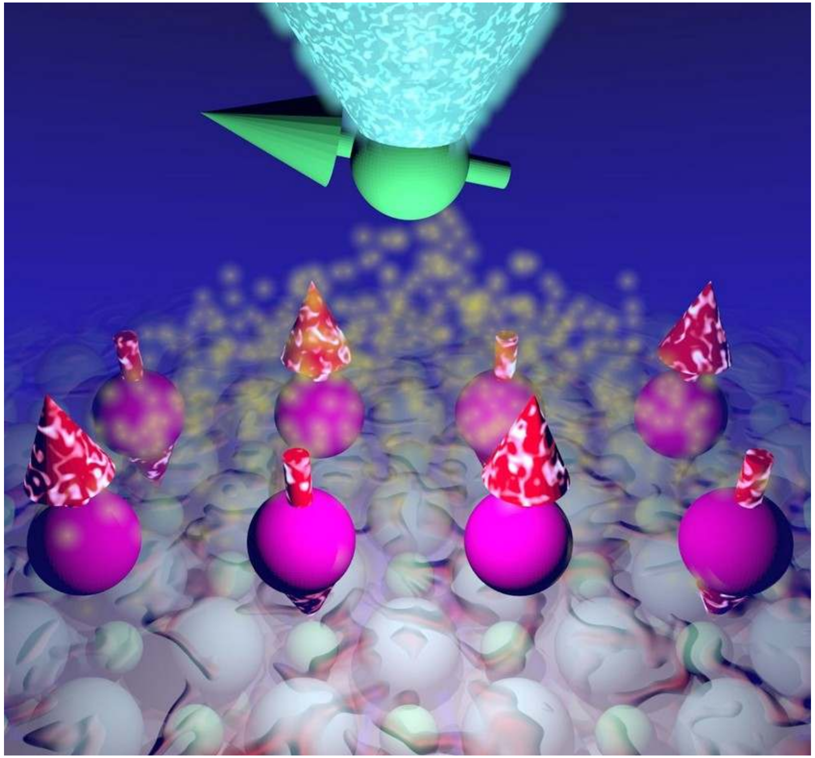


# Statistics of the theoretical model



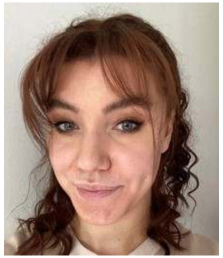

**2D arrays have the largest width of the spin excitation**

# Hamiltonian learning nanoscale magnets



**Hamiltonian learning nanoscale magnets**

Netta Karjalainen



Zina Lippo

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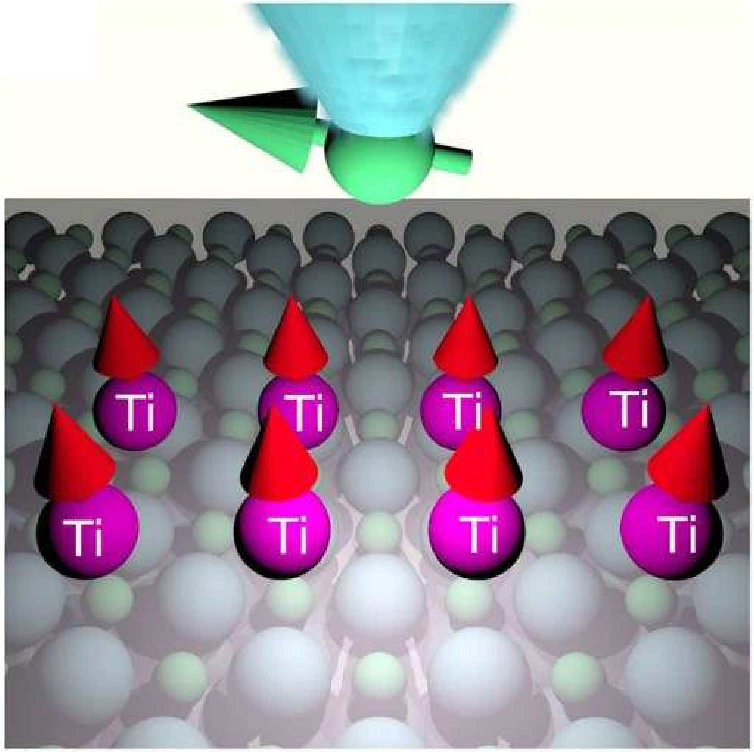
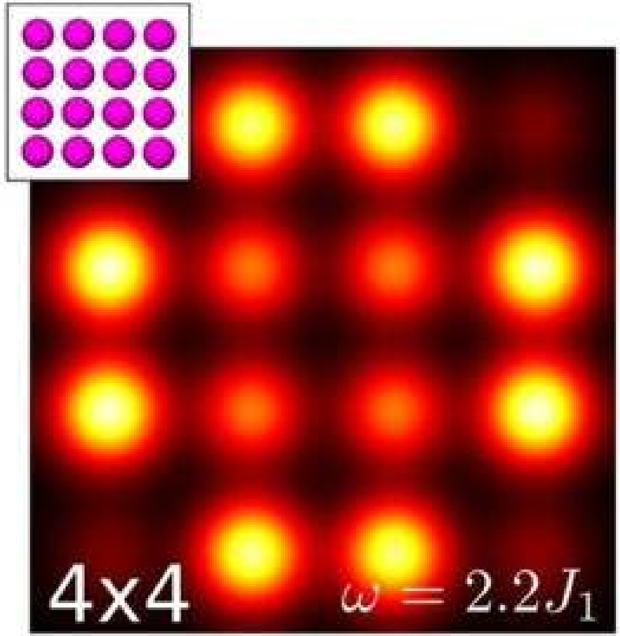
Phys. Rev. Applied 20, 024054 (2023)

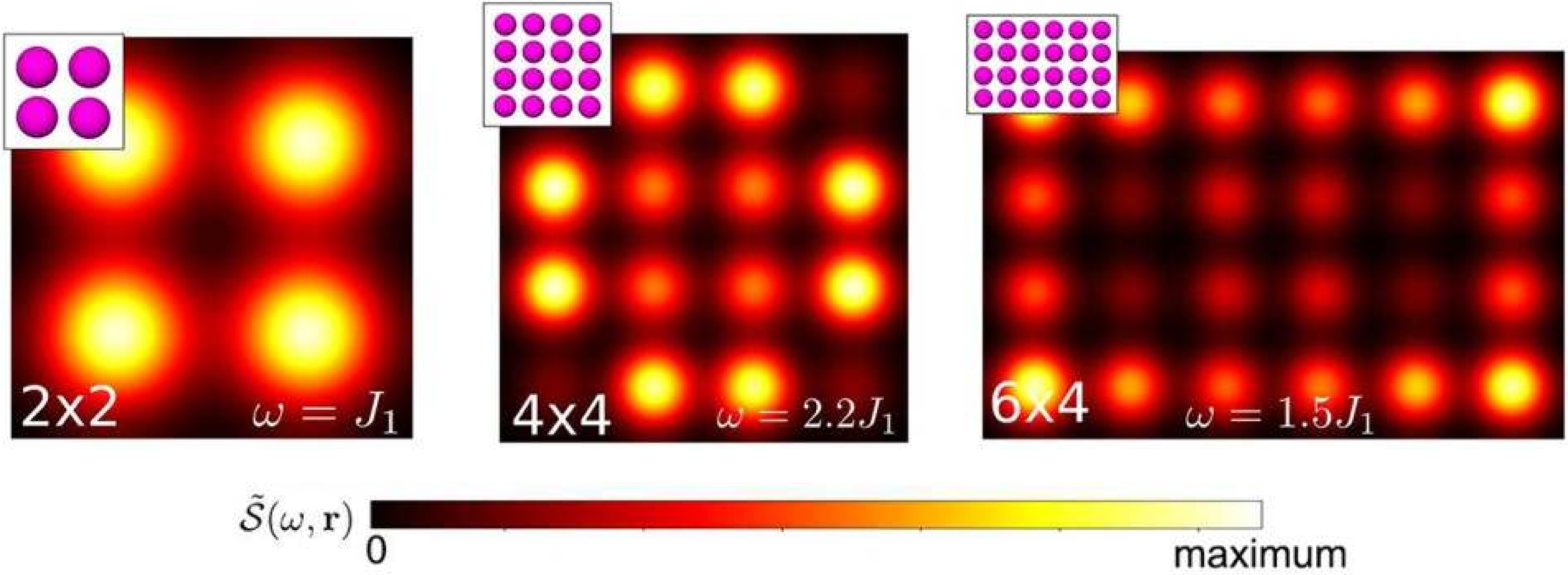
# Spatially resolved excitations



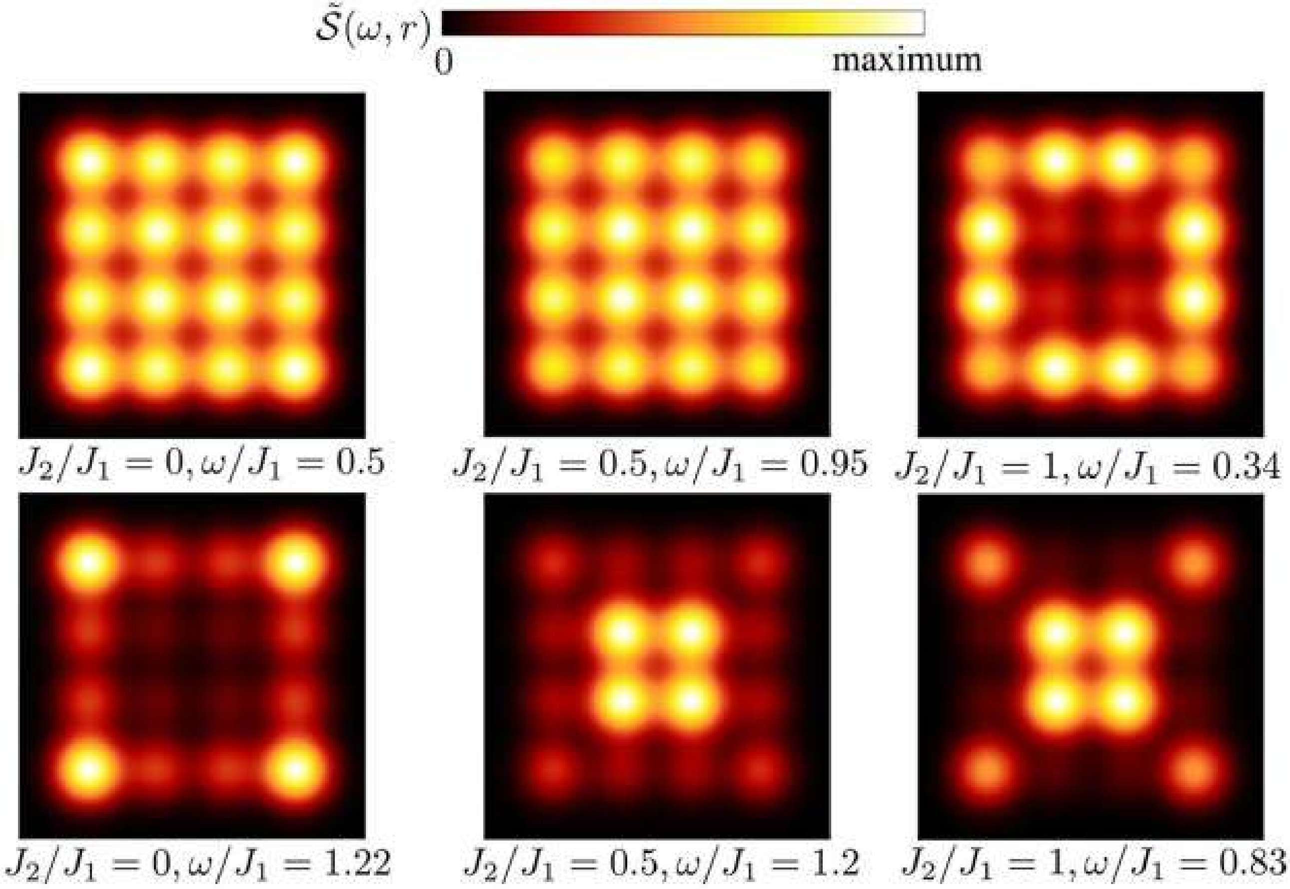

***What can we learn from the Hamiltonian using real-space information?***

# Spatially resolved excitations



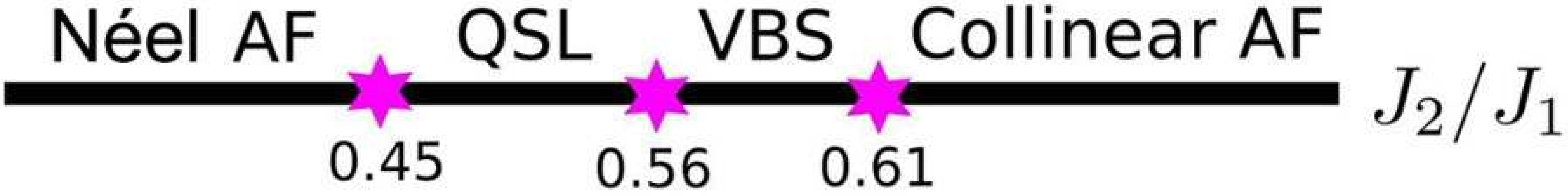

***Spin excitations behave like particle in a box states***

# Spin excitation modes in spin islands



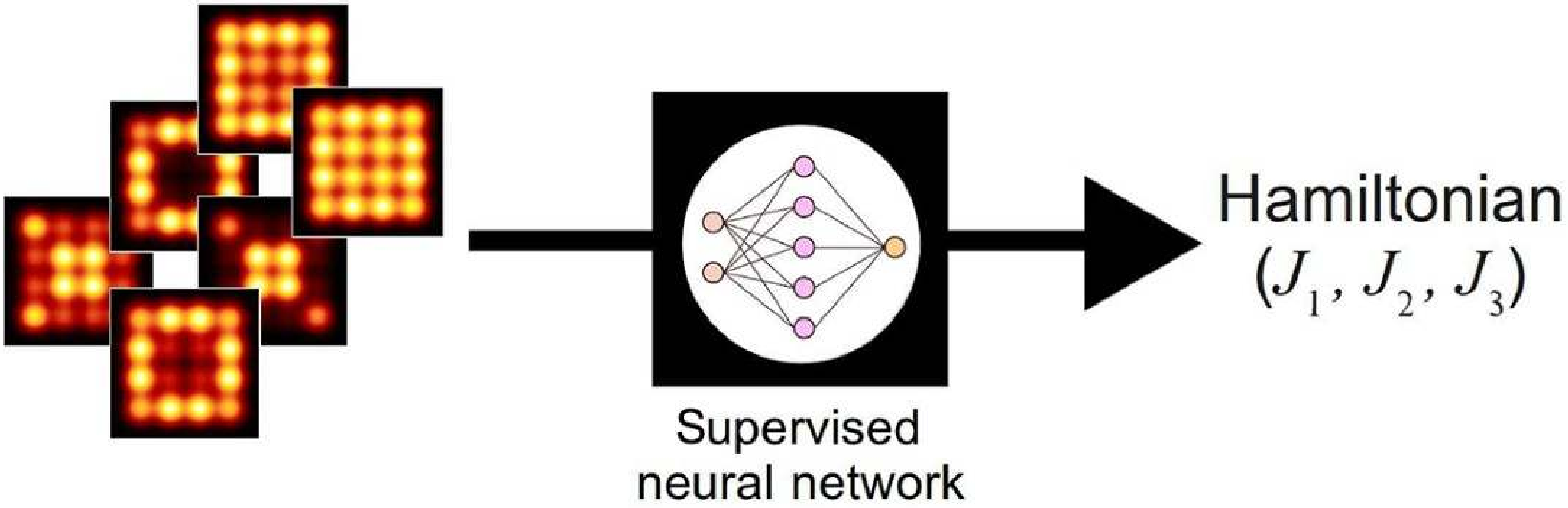
# The extended Heisenberg model

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




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

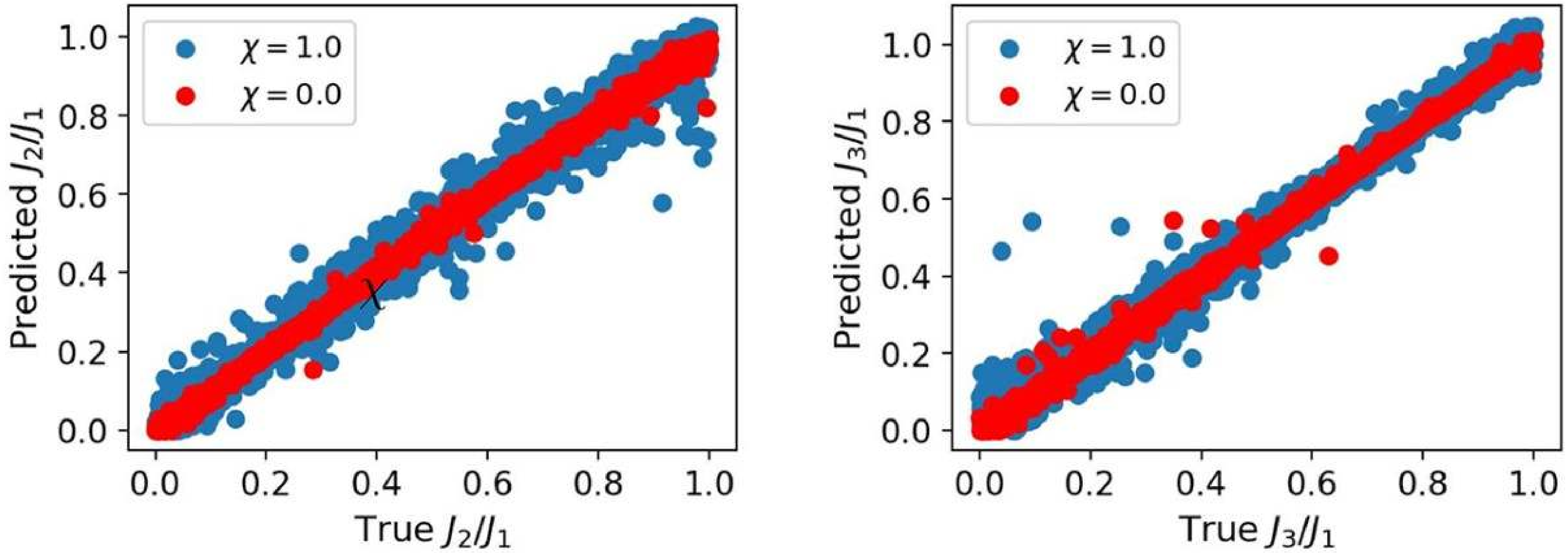
# The idea of Hamiltonian learning




**Provide the spectroscopy as input, obtain the Hamiltonian as output**

# Real VS predicted exchange parameters

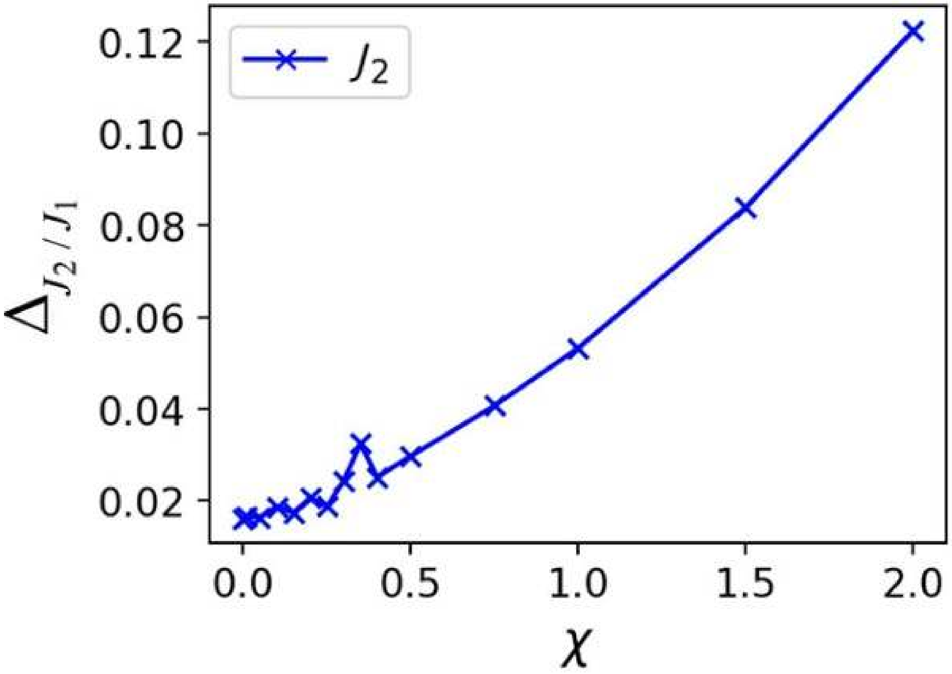
With noise $$\mathcal{S}(\omega, \mathbf{r}_i)_{\text{noisy}} = \mathcal{S}(\omega, \mathbf{r}_i) \cdot |1 + \zeta(\omega)| \quad \zeta(\omega) \in [-\chi, \chi]$$

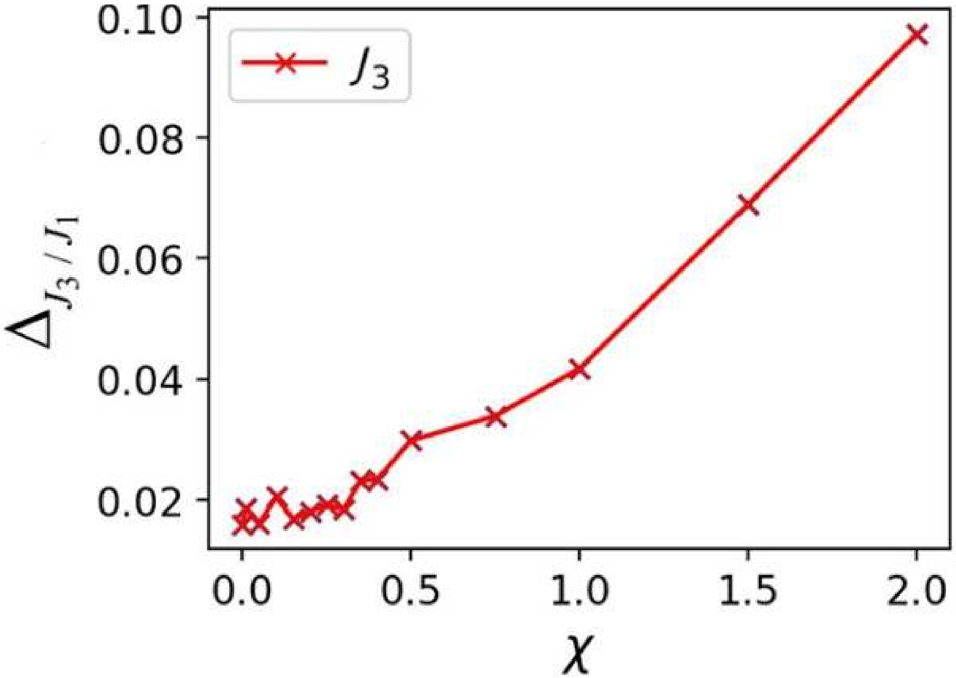



***A supervised learning algorithm extracts faithfully the exchange parameters***

# Predictions with noise

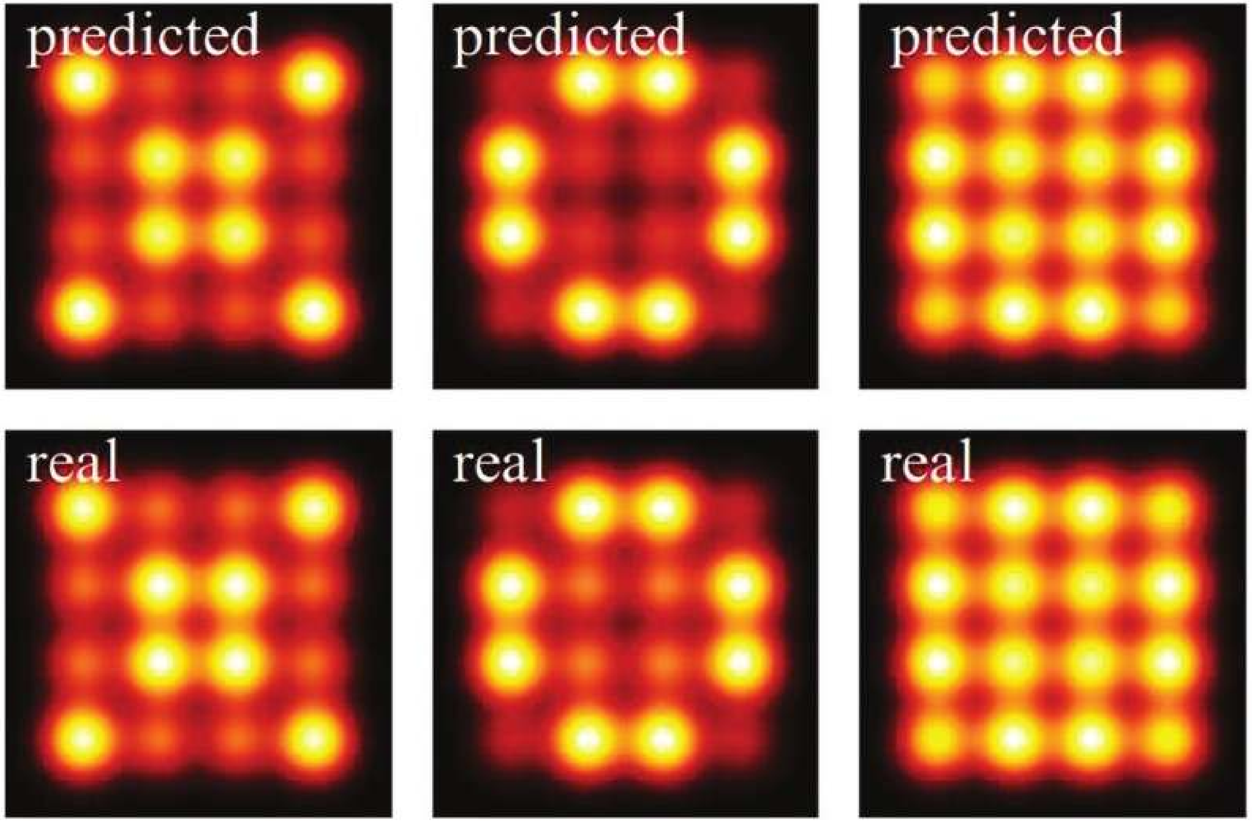
$$\mathcal{S}(\omega, \mathbf{r}_i)_{\text{noisy}} = \mathcal{S}(\omega, \mathbf{r}_i) \cdot |1 + \zeta(\omega)| \qquad \zeta(\omega) \in [-\chi, \chi]$$



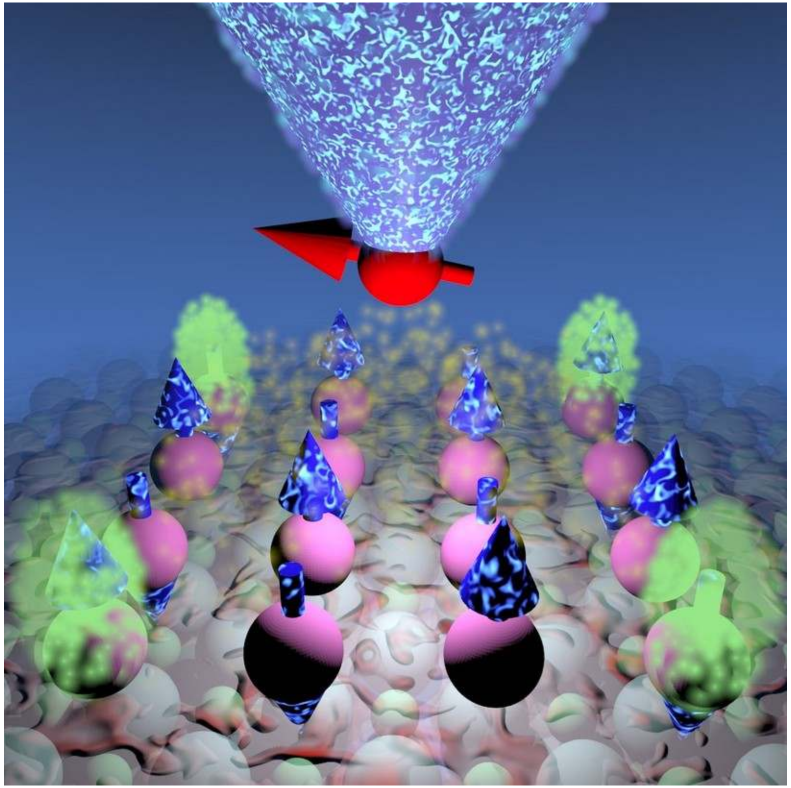




***Quality of prediction remain good with sizable noise levels***

# 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

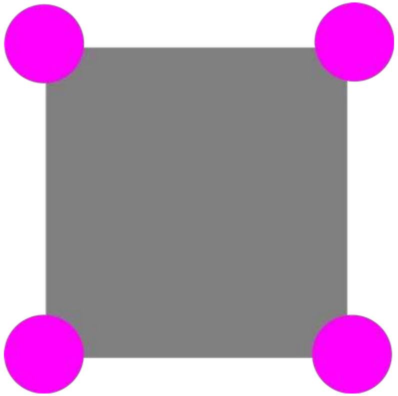
# Topological quantum magnets

**First order topological quantum magnet**

1D gaped bulk
0D fractional edge modes

*Nature 598, 287–292 (2021)*

**Second order topological quantum magnet**



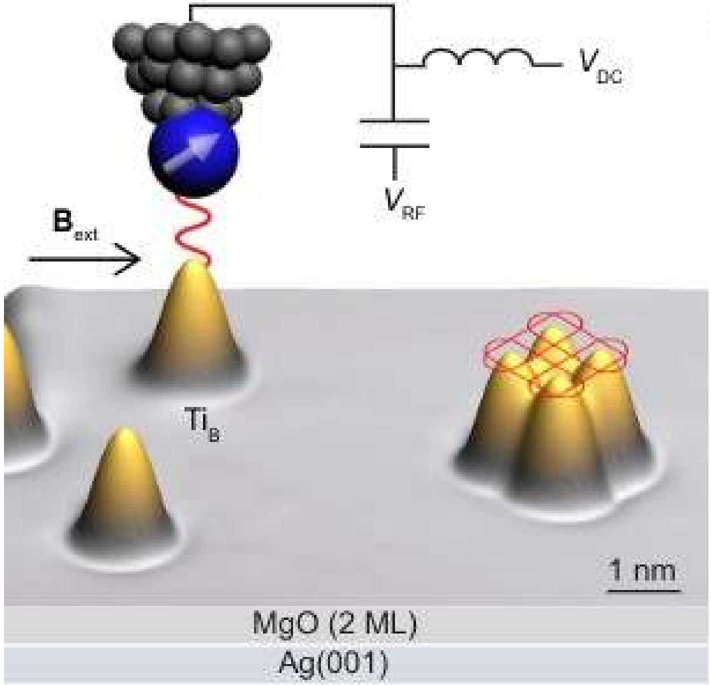
2D gaped bulk
0D fractional edge modes

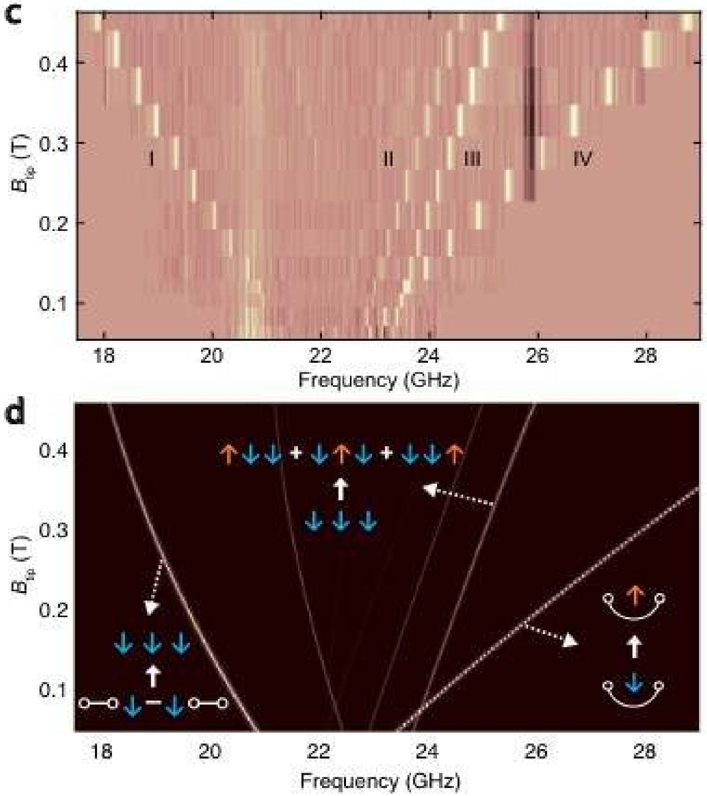
*Nature Nanotechnology (2024)*

*10.1038/s41565-024-01775-2*

# Artificial spin models with Ti@MgO

Ti@MgO (2x2 lattice)

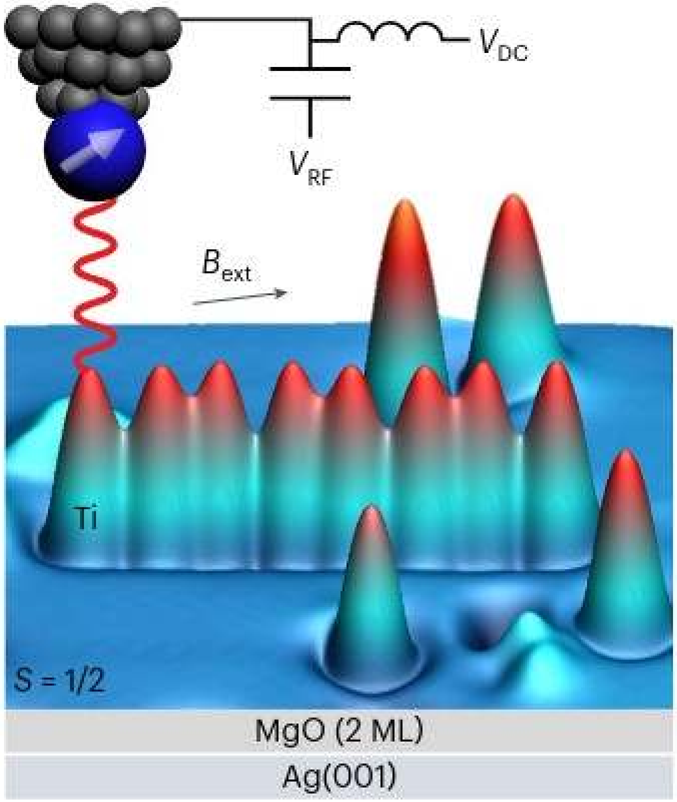


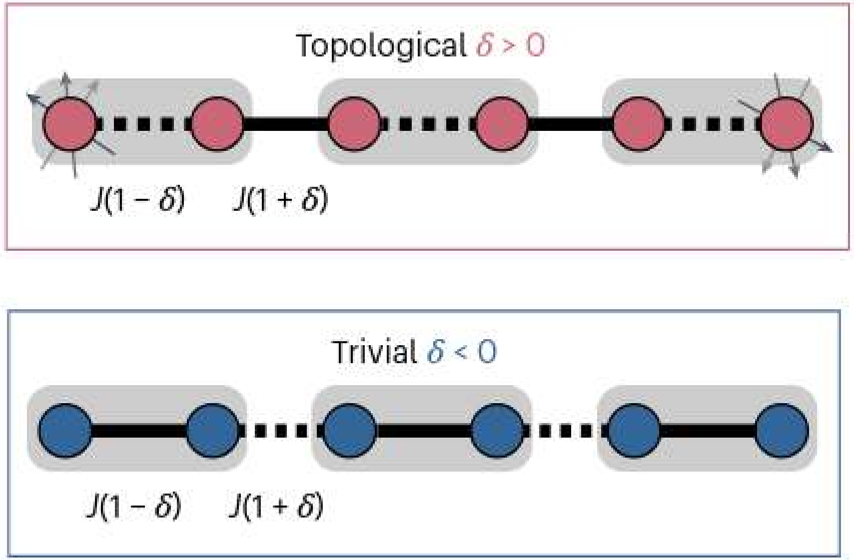

Nature Communications 12, 993 (2021)

**Can we create new states of matter?**

# First order topological quantum magnets



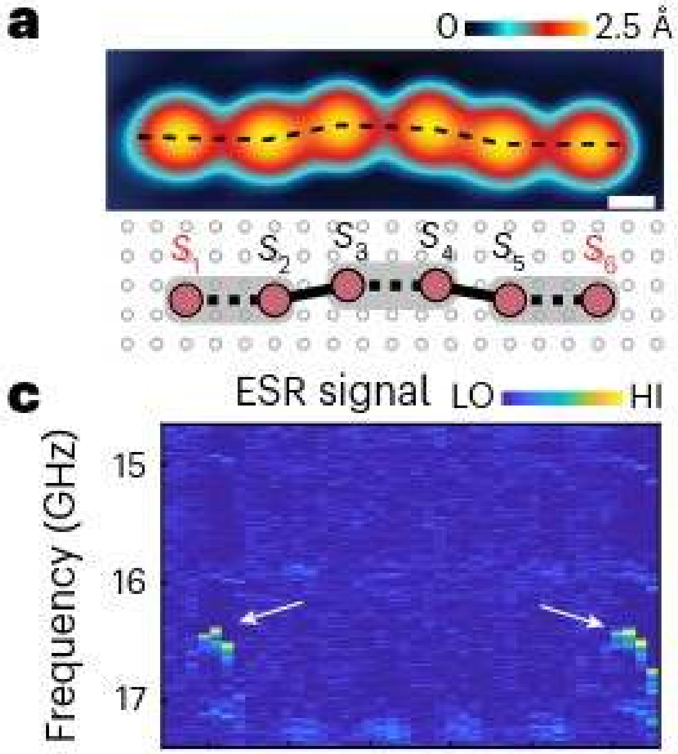

**Two possible configurations**



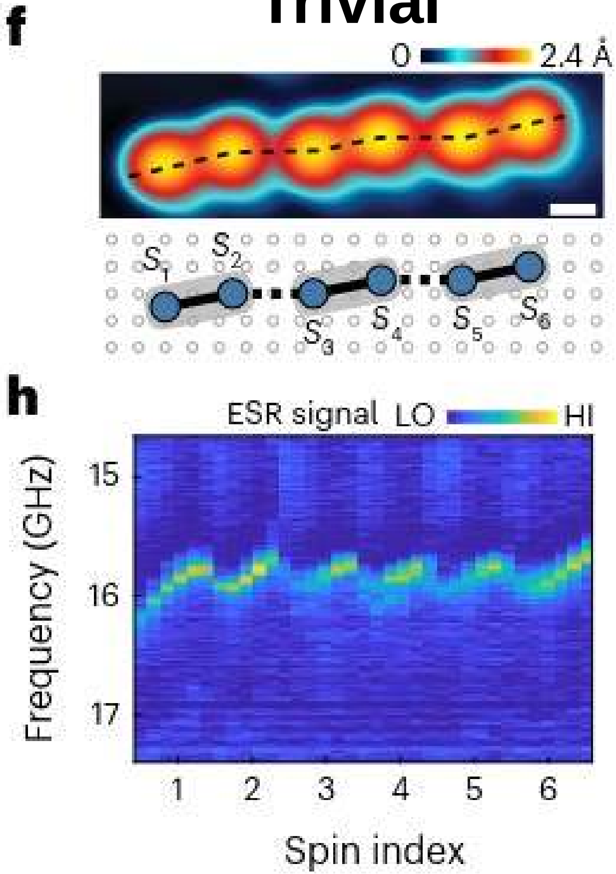

Nature Nanotechnology (2024)
10.1038/s41565-024-01775-2

# First order topological quantum magnets

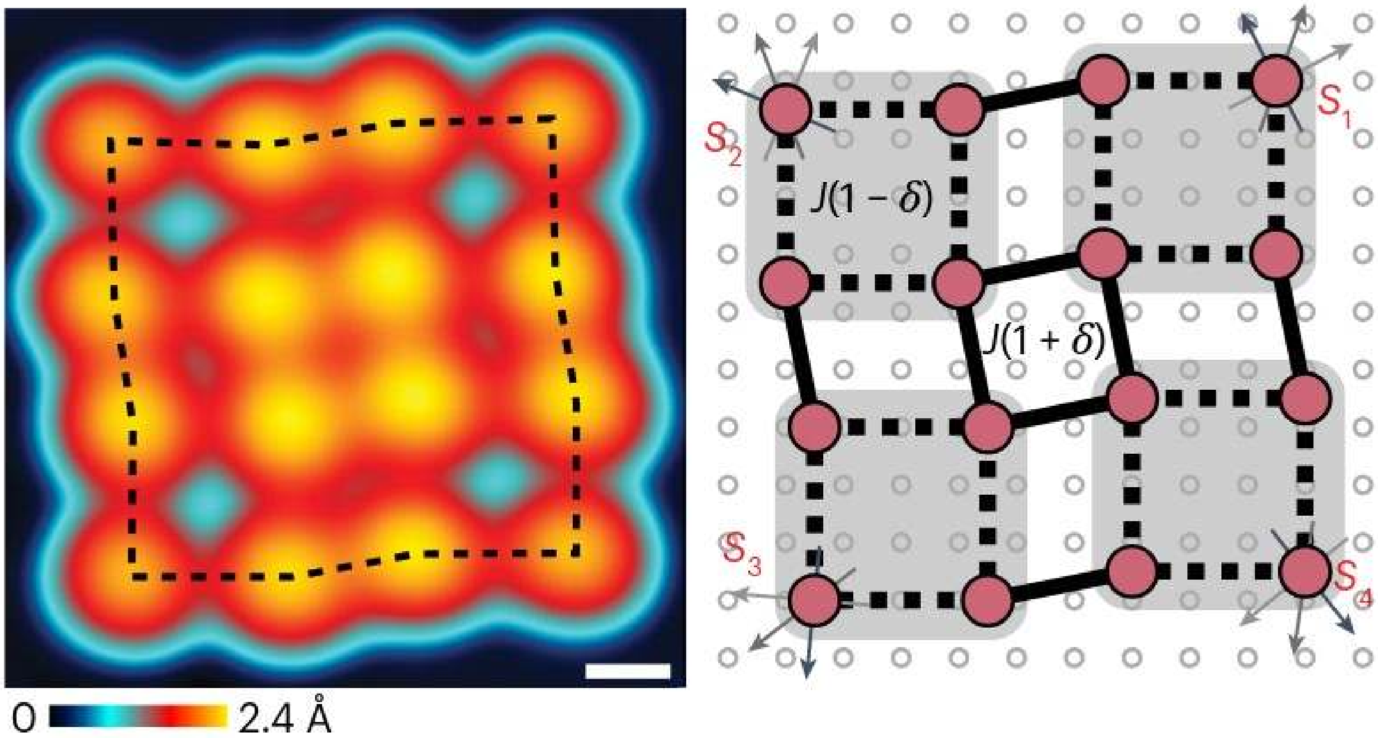
**Topological**




**Trivial**

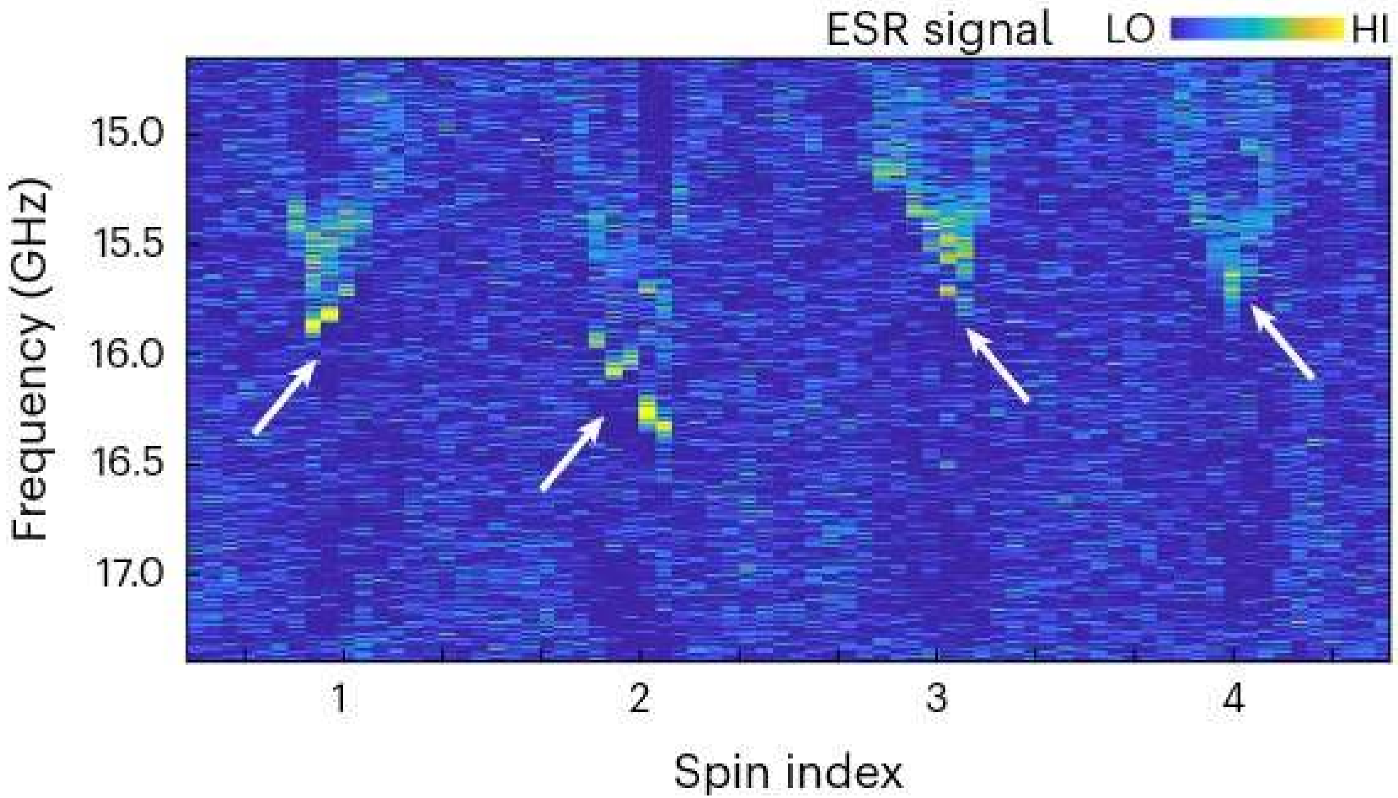


# A higher order topological quantum magnet




**The higher order topological quantum magnet shows topological corner modes**

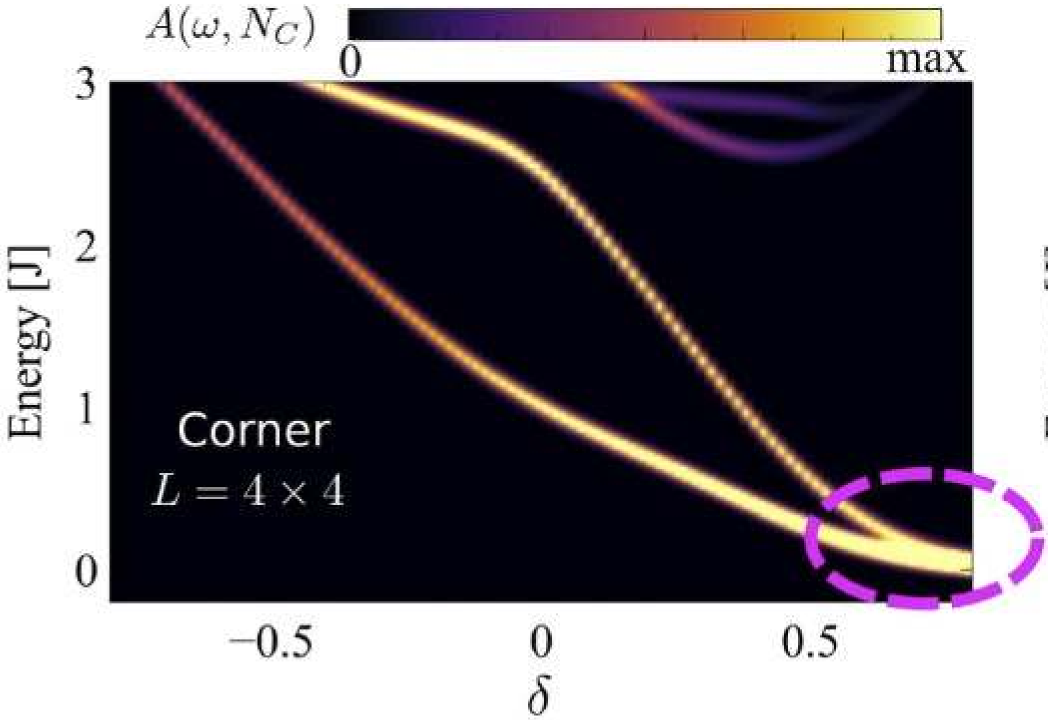
# A higher order topological quantum magnet



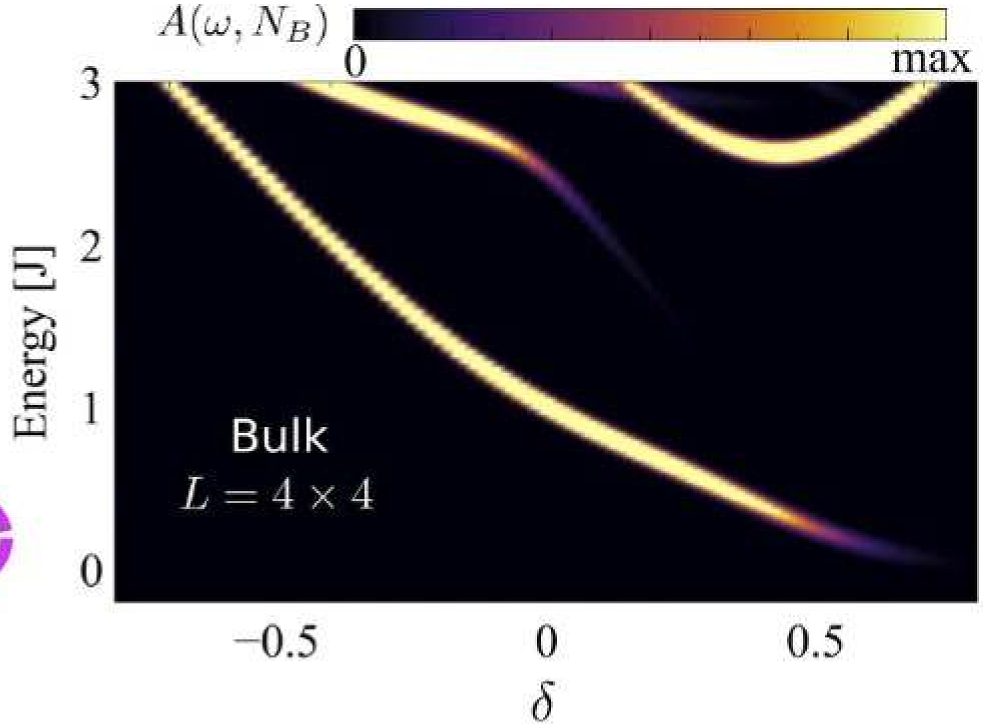

***Topological corner modes are measured coexisting with a bulk spectral gap***

# A higher order topological quantum magnet

**Corner spin excitations**

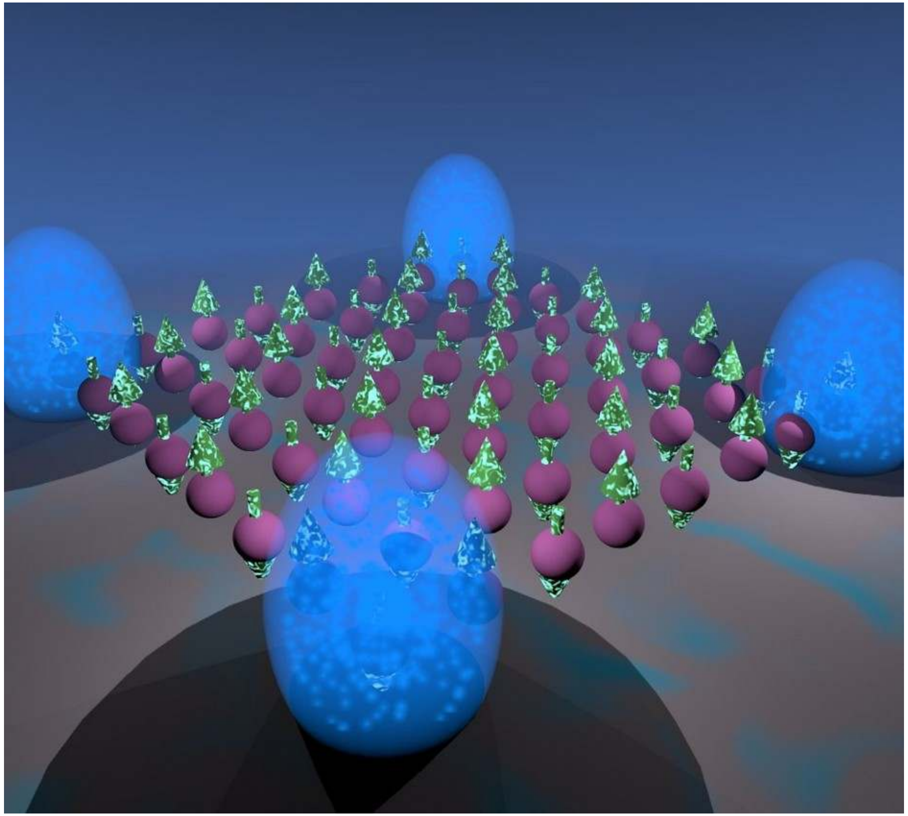



**Bulk spin excitations**

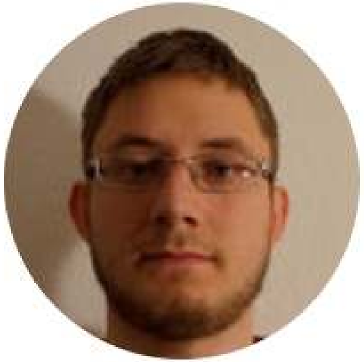



**The tetramerization of the lattice creates topological corner spin excitations**

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

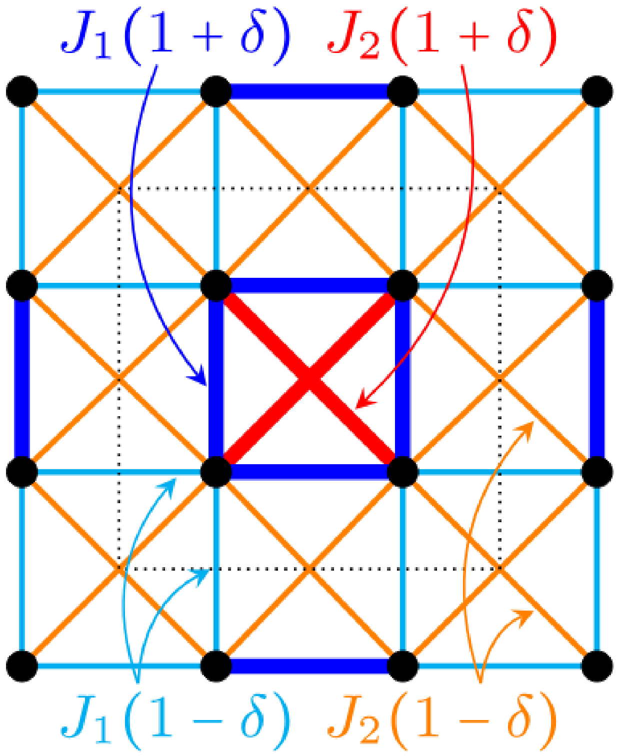


Pascal Vecsei

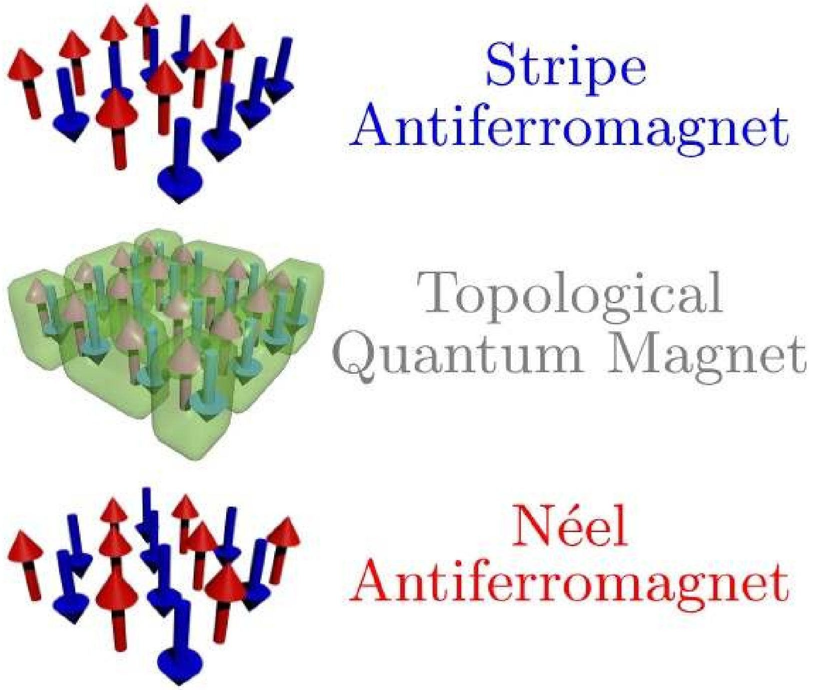


arXiv:2408.16453 (2024)

# The model of a frustrated topological quantum magnet




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

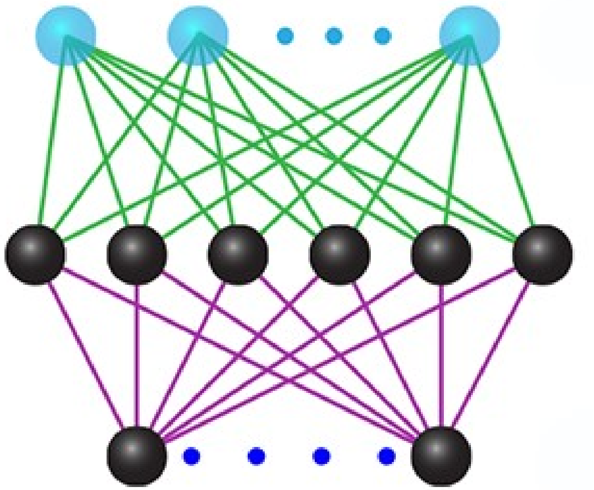


# Solving frustrated quantum 2D models

## Tensor-networks


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

## Neural-network quantum states

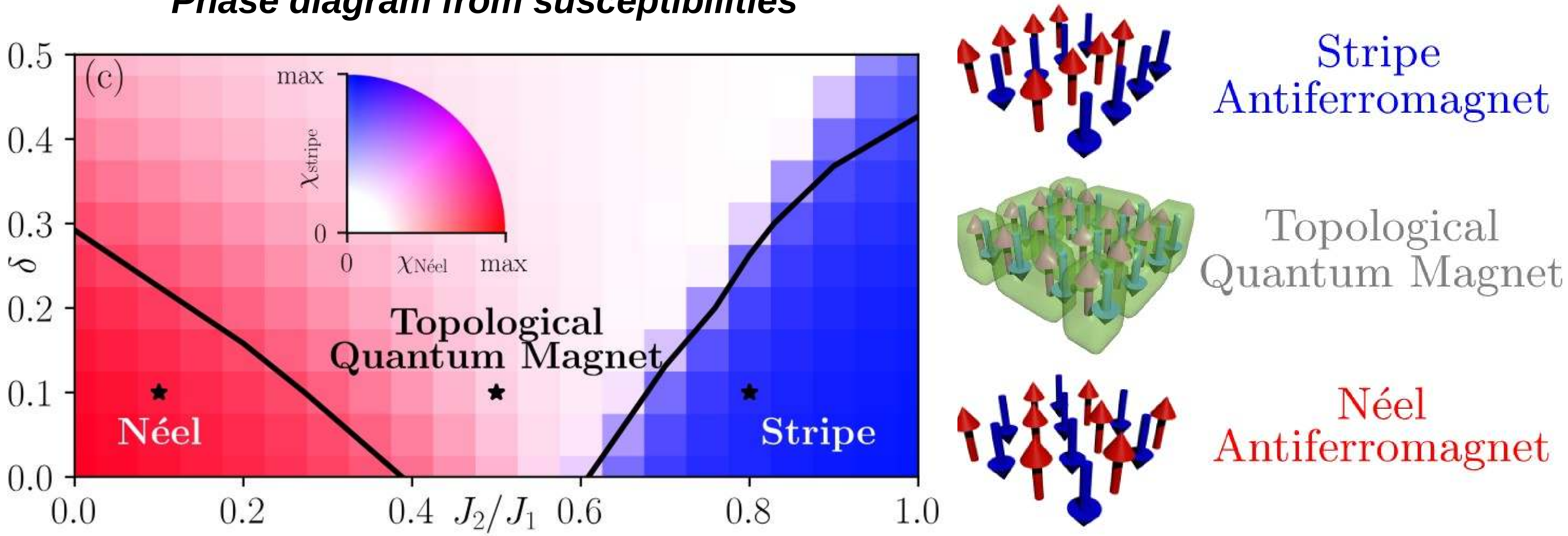


*Science 355.6325 (2017): 602-606.*

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

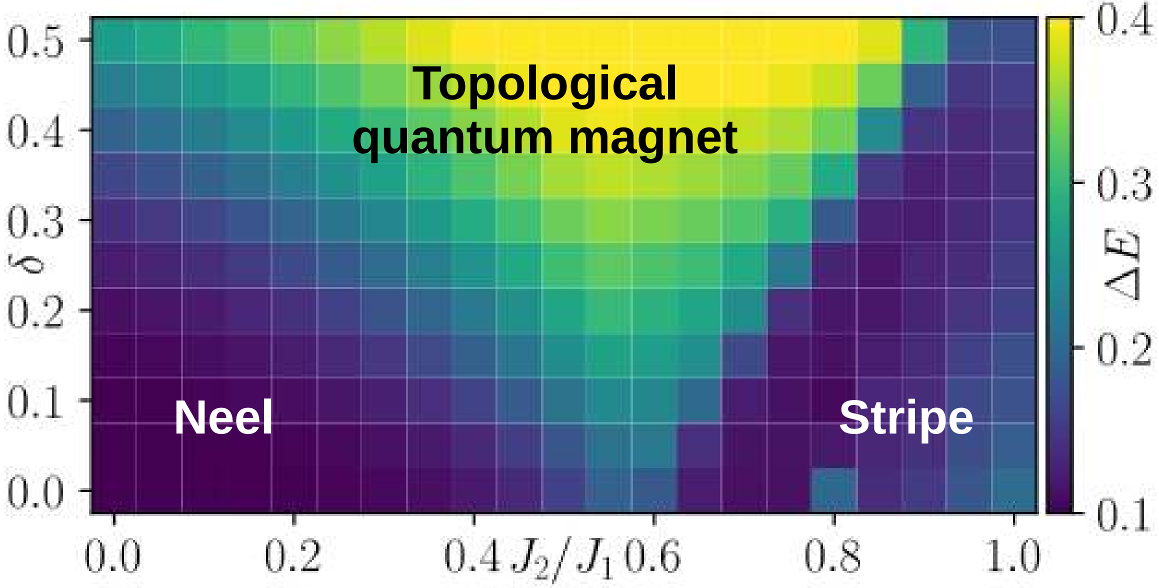
# The phase diagram of the higher order topological quantum magnet

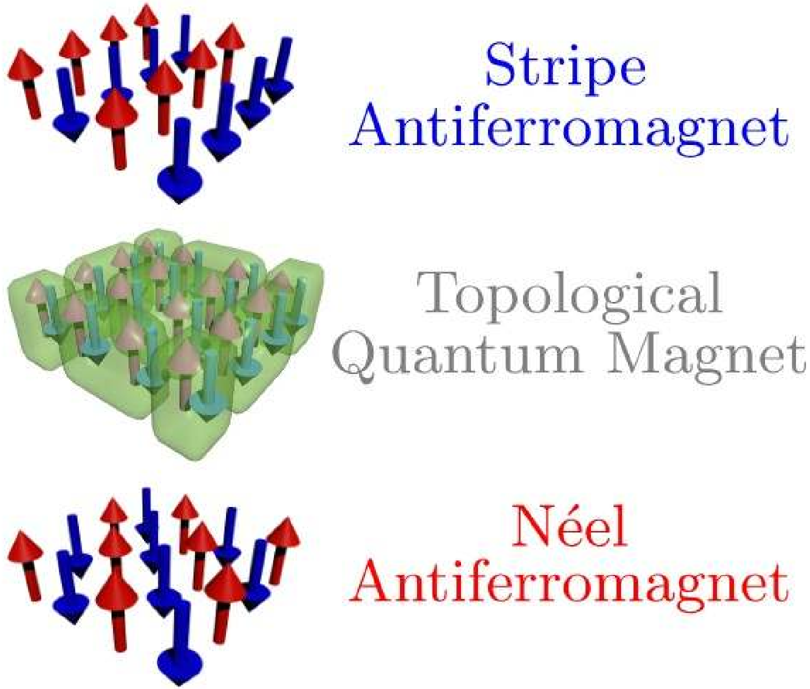
***Phase diagram from susceptibilities***



# 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

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

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

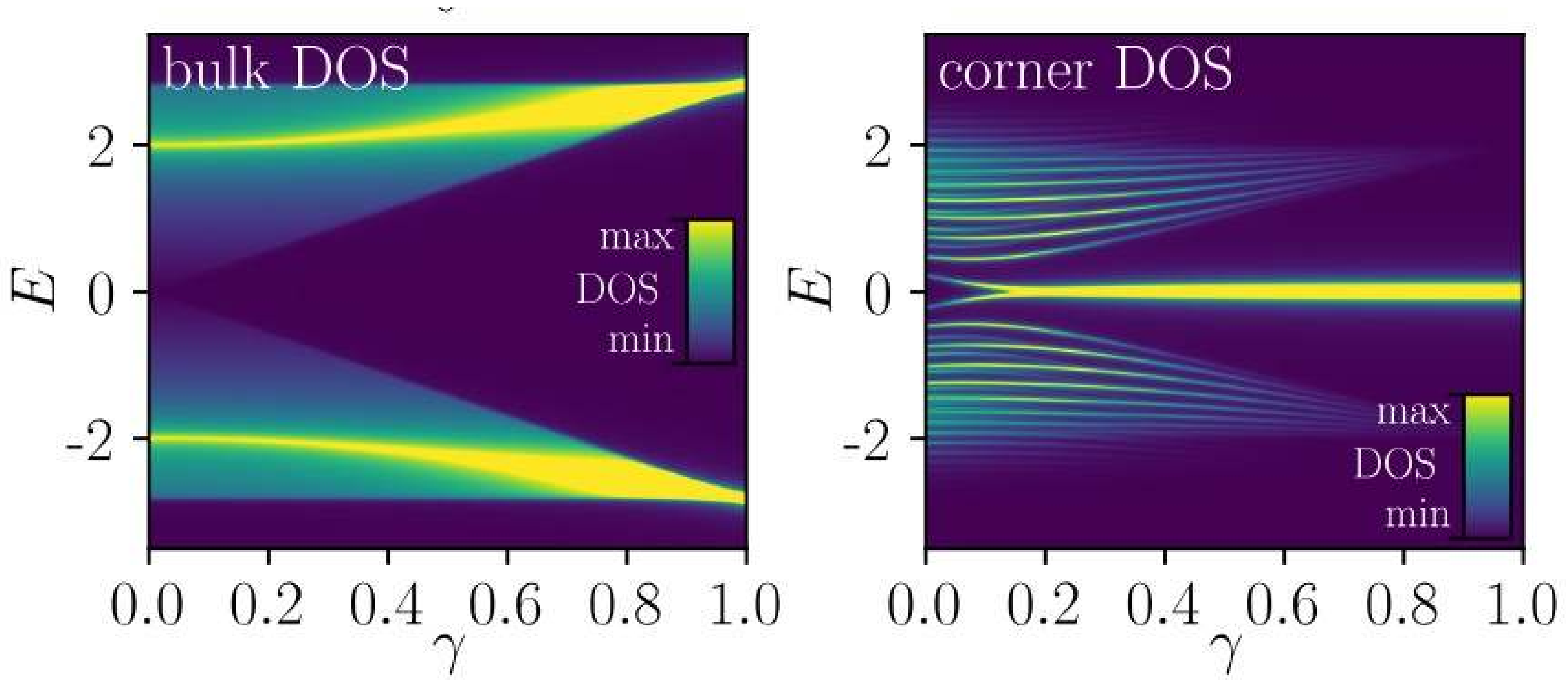
**Spinon pi-flux model**

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

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

*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

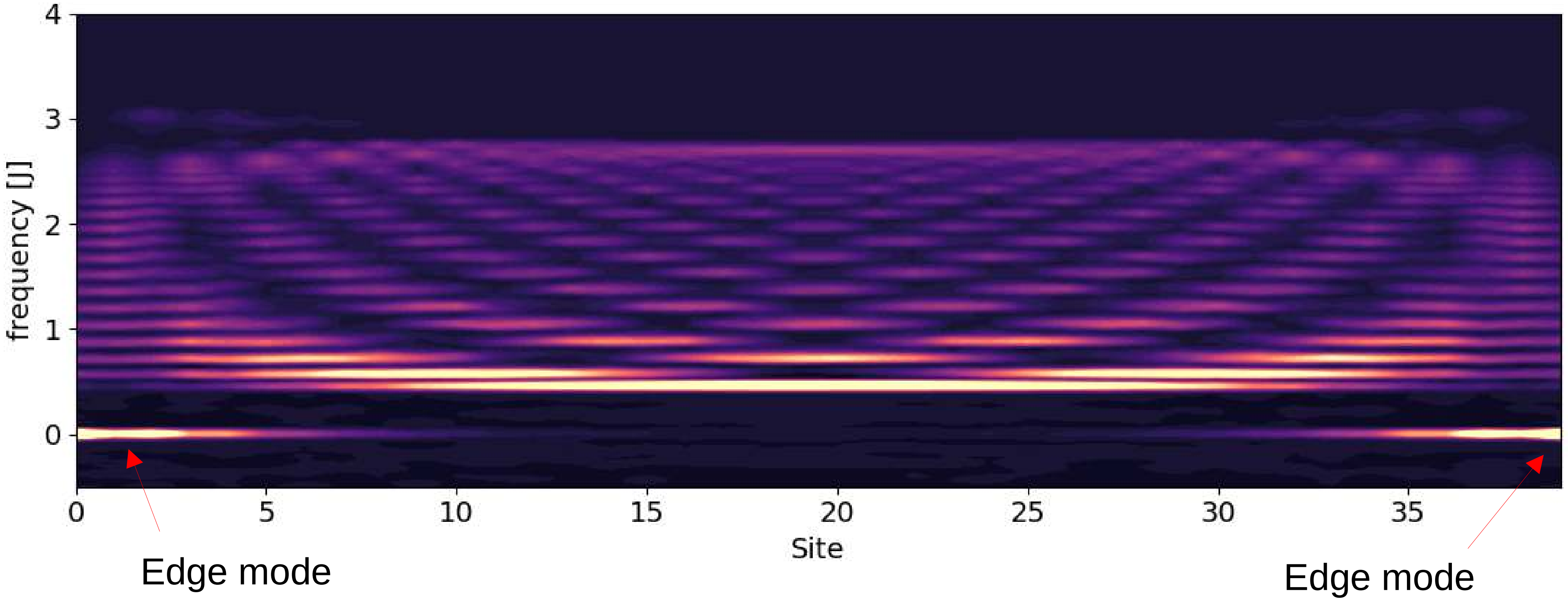
*Python library for tensor-network kernel polynomial algorithms for spins, fermions, parafermions, with static solvers for Hermitian and non-Hermitian modes*

```
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

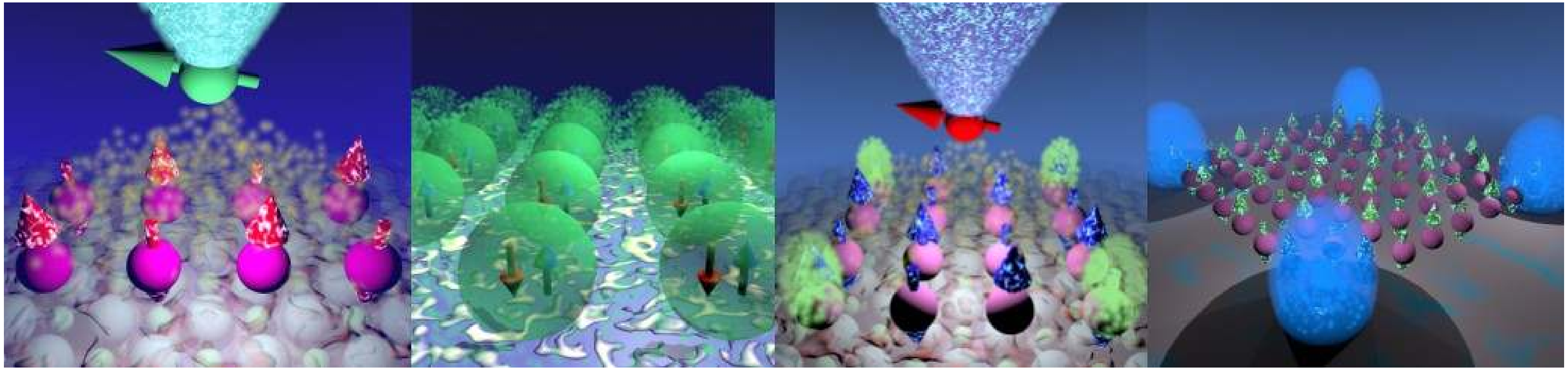
# Open-source software for many-body quantum magnets

**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**