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

Jose Lado

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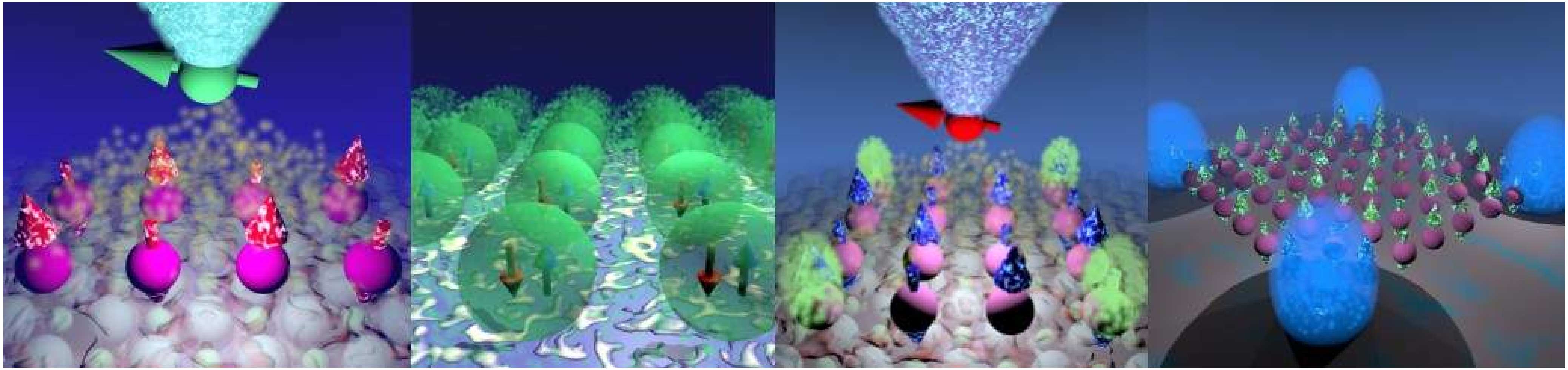


Phys. Rev. Appl 20, 024054 (2023)

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

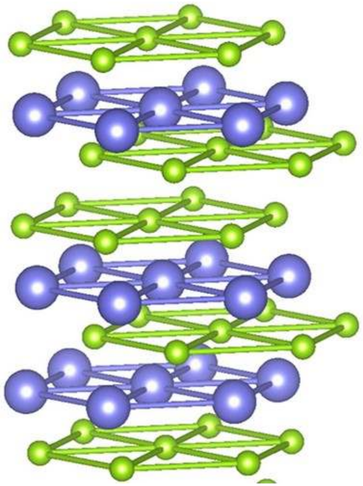
Nature Nano (2024)

arXiv:2408.16453 (2024)

JQUEST: Quantum Electronics, Superconductivity, and Topology workshop., University of Jyväskylä, Finland
December 5th 2024

Emergence in quantum materials

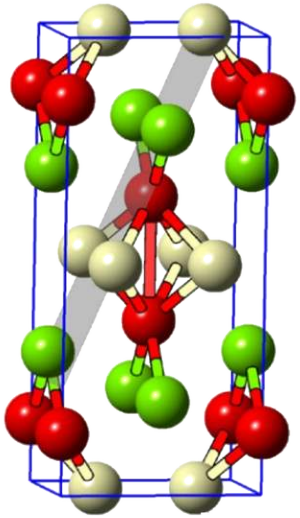
Topological materials



Bi_2Se_3

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

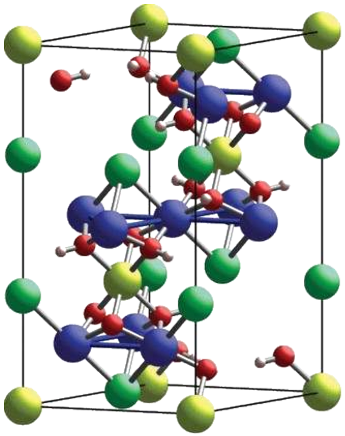
Unconventional superconductors



UTe_2

Nature 579, 523–527 (2020)

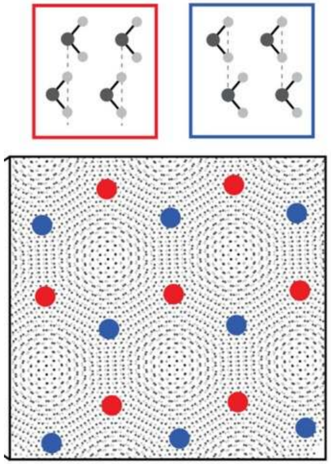
Quantum spin liquids



$ZnCu_3(OH)_6Cl_2$

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

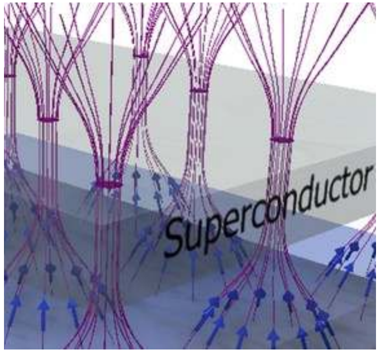
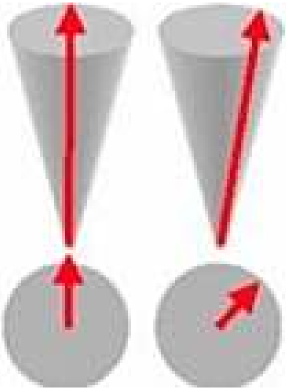
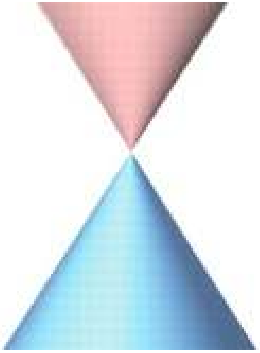
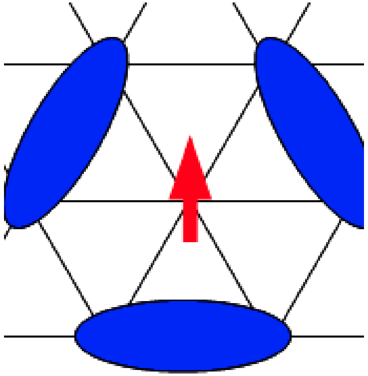
Fractional topological matter



Twisted $MoTe_2$

Nature 622, 63–68 (2023)

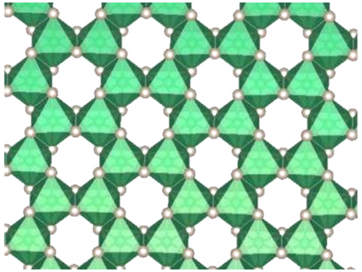
Emergent excitations in quantum materials

Vortexes	Magnons	Skyrmions	Dirac fermions	Spinons
				
Superconductors	***Ordered magnets***	**Non-collinear magnets**	***Topological materials***	***Quantum spin liquids***

The discovery of new quasiparticles opens new possibilities in quantum technologies

Magnetic quantum materials

Ferromagnet, antiferromagnets

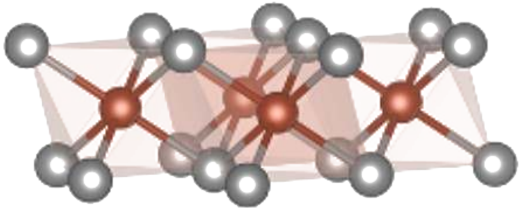


CrI_3, $CrCl_3$, $CrBr_3$

Nature 546, 270–273 (2017)

Break time-reversal

Multiferroics

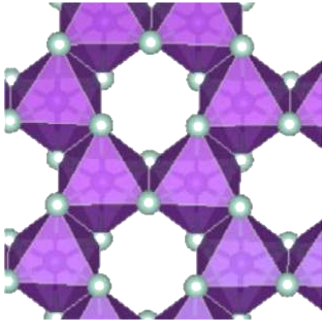


NiI_2

Nature 602, 601–605 (2022)

Break time-reversal
and inversion symmetry

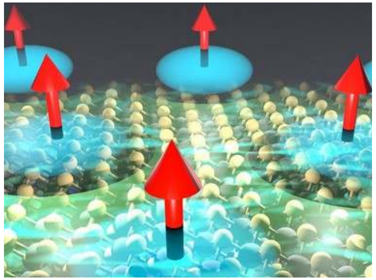
(proximal) Quantum spin-liquids



$RuCl_3$, 1T-TaS_2

Nature Physics 17, 1154–1161 (2021)

Heavy-fermion Kondo insulators



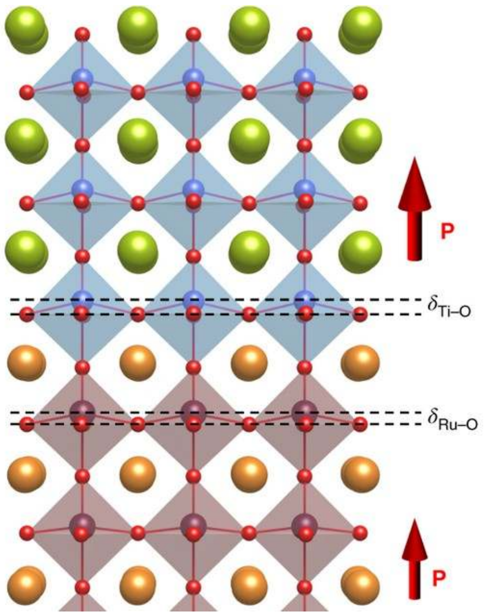
1T-TaS_2/1H-TaS_2

Nature 599, 582–586 (2021)

Do not break time-reversal

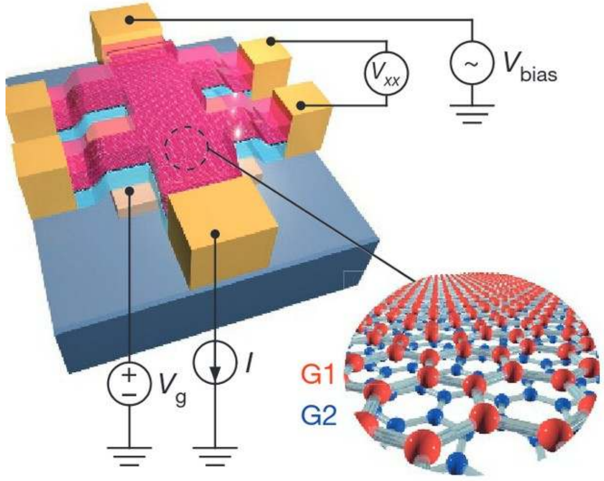
Artificial quantum materials

Oxide interfaces



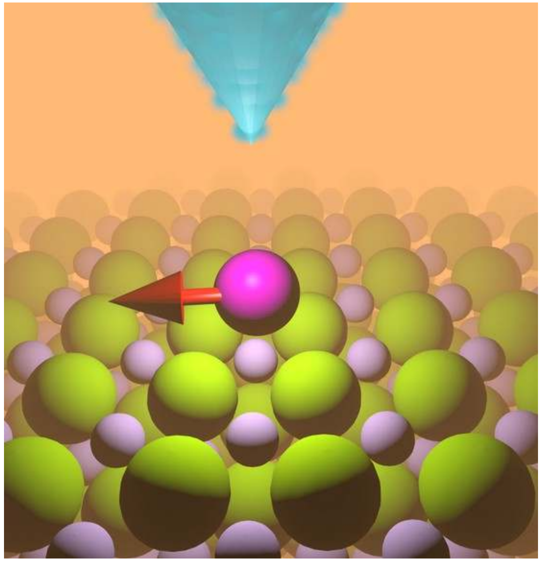
Nature Materials 17, 1087–1094 (2018)

Twisted van der Waals materials



Nature 556 43–50 (2018)
Nature 588, 424–428 (2020)
Nature 622, 63–68 (2023)

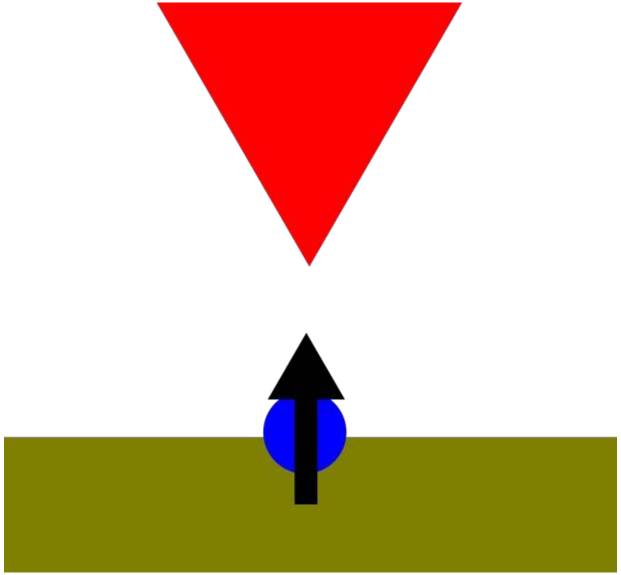
Atomic lattices



Nature Physics 12 (7), 656 (2016)
Nature Physics 13 (7) 668 (2017)
Science 335 (6065), 196-199 (2012)

Two ways of measuring spin-excitations in atomic-scale magnets

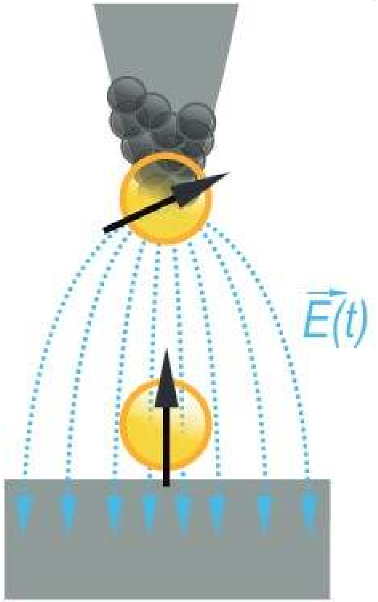
Inelastic spectroscopy



Science 306 (5695), 466-469 (2004)

Without spin-polarized tip

Electrically driven paramagnetic resonance

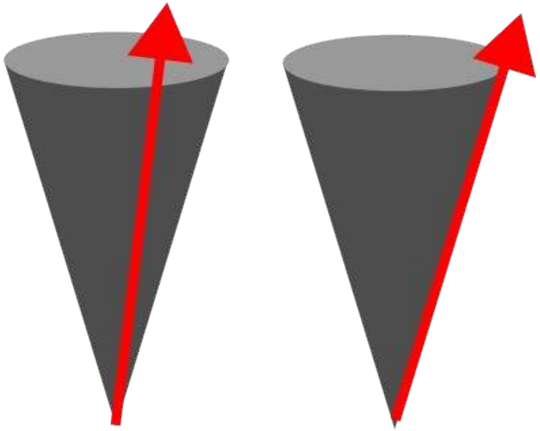


Science 350 (6259), 417-420 (2015)

With spin-polarized tip

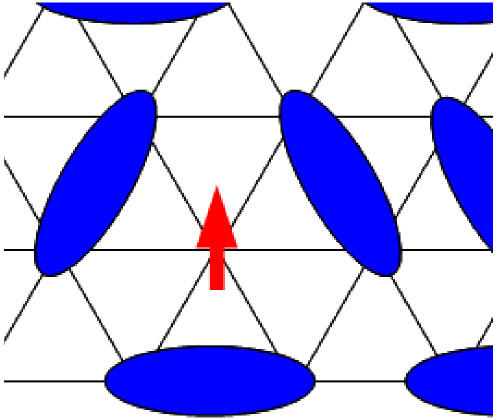
Excitations in atomic-scale magnets

Magnons



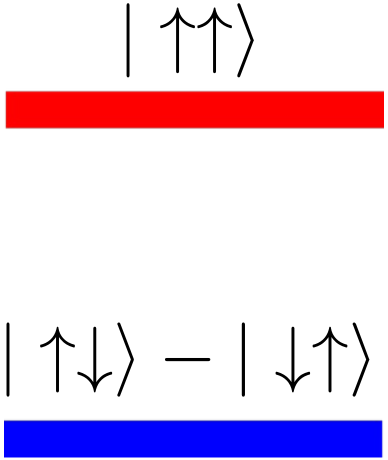
S=1

Spinons



S=1/2

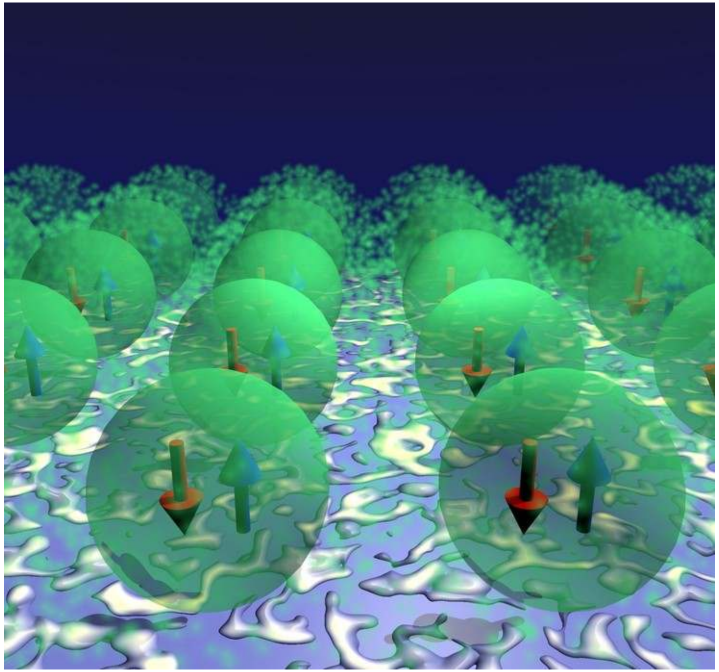
Triplons



S=1

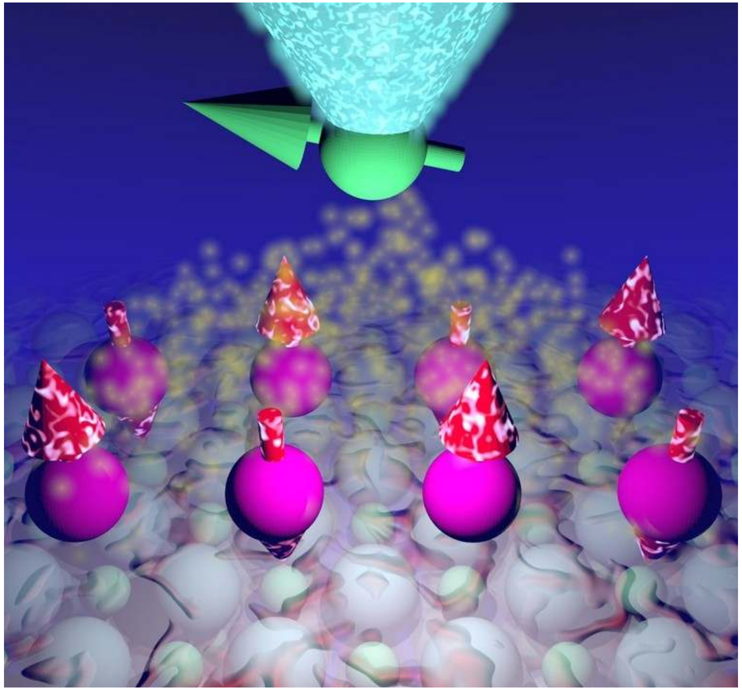
Plan for today

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

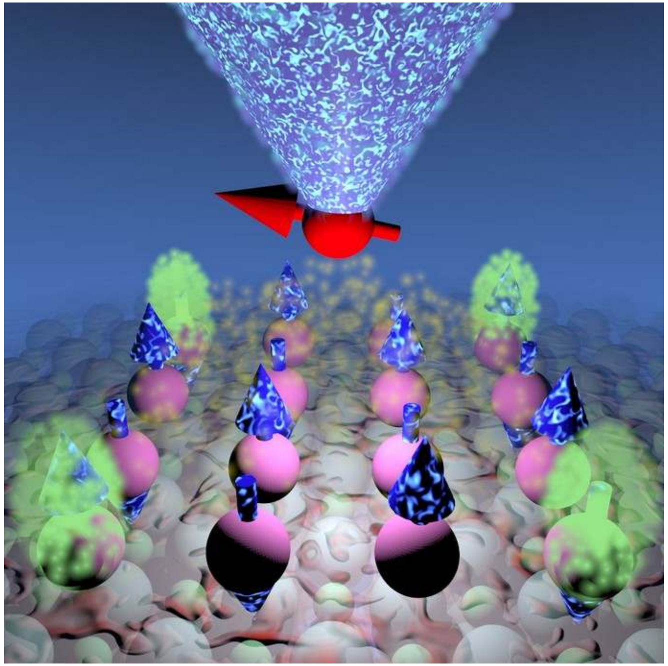
Guangze Chen

Adolfo Fumega

Phys. Rev. Applied 20, 024054 (2023)

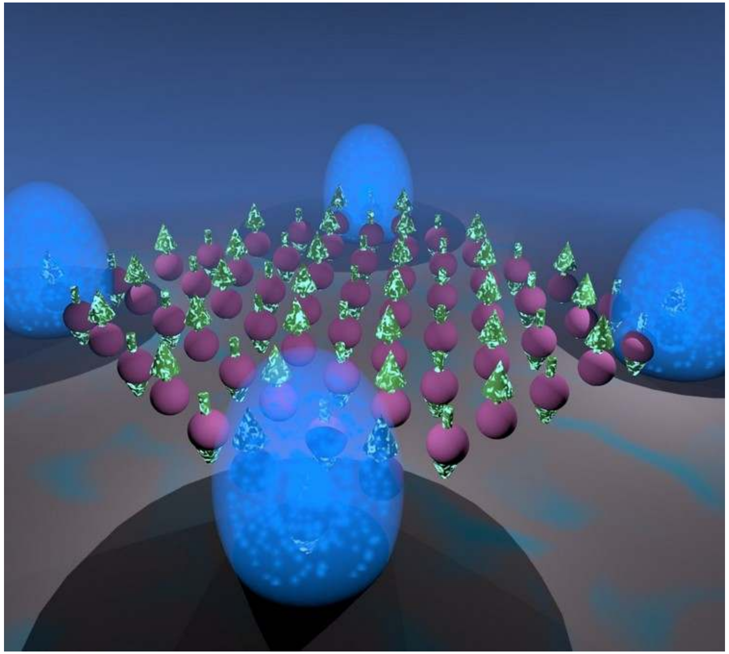
Plan for today

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

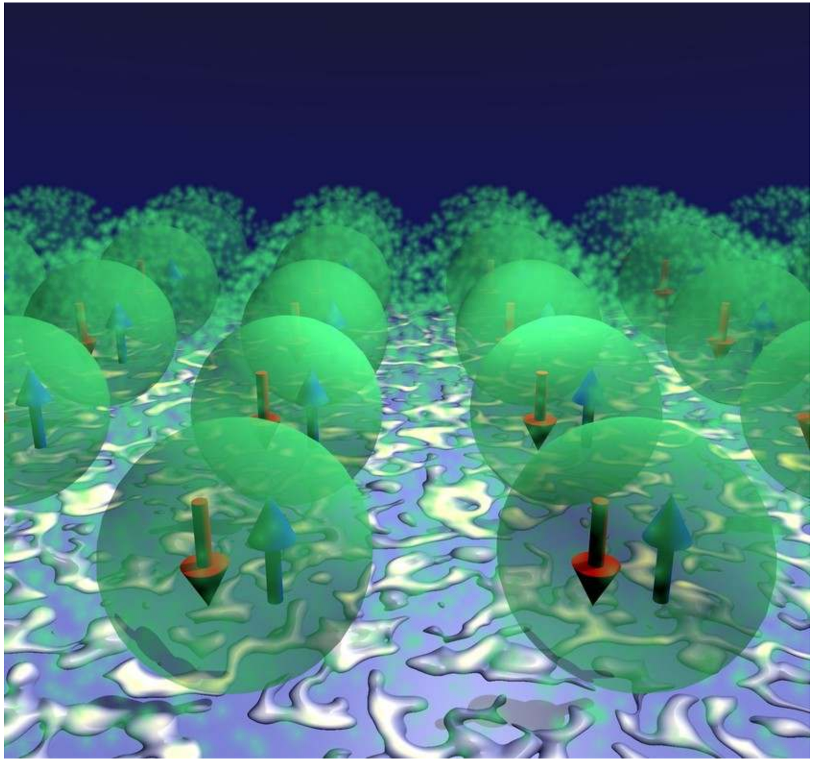
Nature Nanotechnology (2024), 10.1038/s41565-024-01775-2

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

The quantum Heisenberg dimer

Let us take a minimal quantum magnet

$$\mathcal{H} = \vec{S}_0 \cdot \vec{S}_1$$

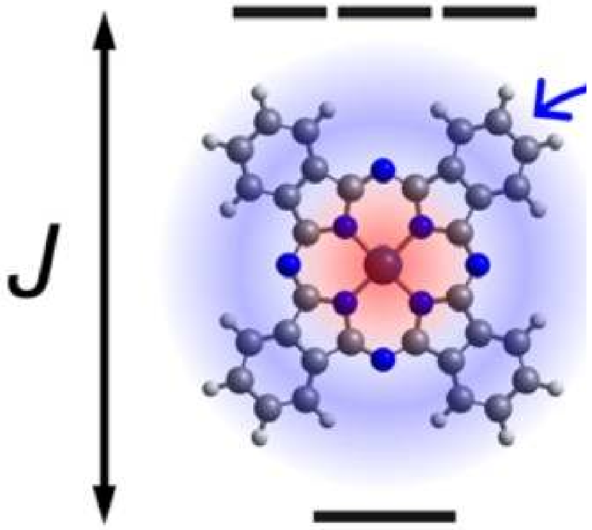
The ground state is unique, and does not break time-reversal

$$|GS\rangle = \frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle] \qquad \langle \vec{S}_i \rangle = 0$$

The state is maximally entangled

How does this generalize to a macroscopic system, and how can we see its quasiparticles?

Triplet excitations in a molecule



S = 1

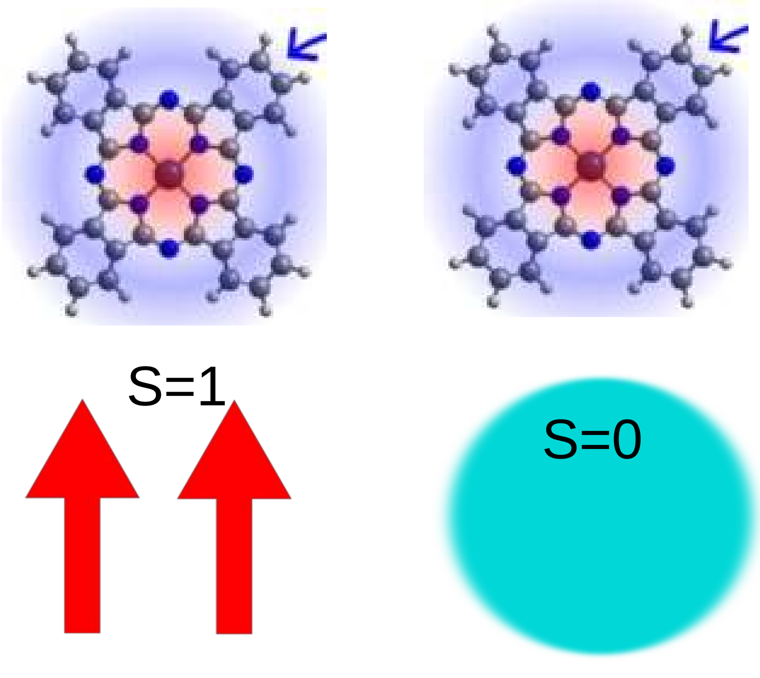
S = 0

Internal antiferromagnetic coupling

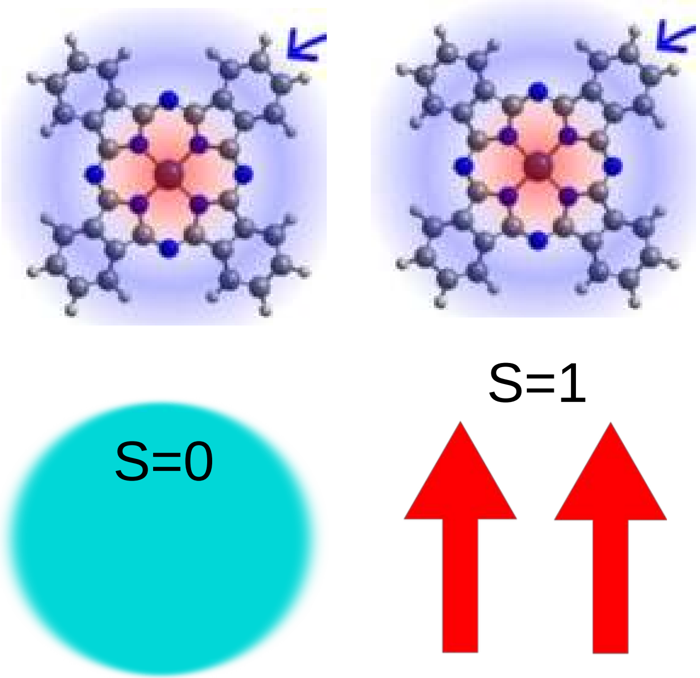
$$H = J\mathbf{S}\cdot\mathbf{K}$$

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

Triplons in a dimer



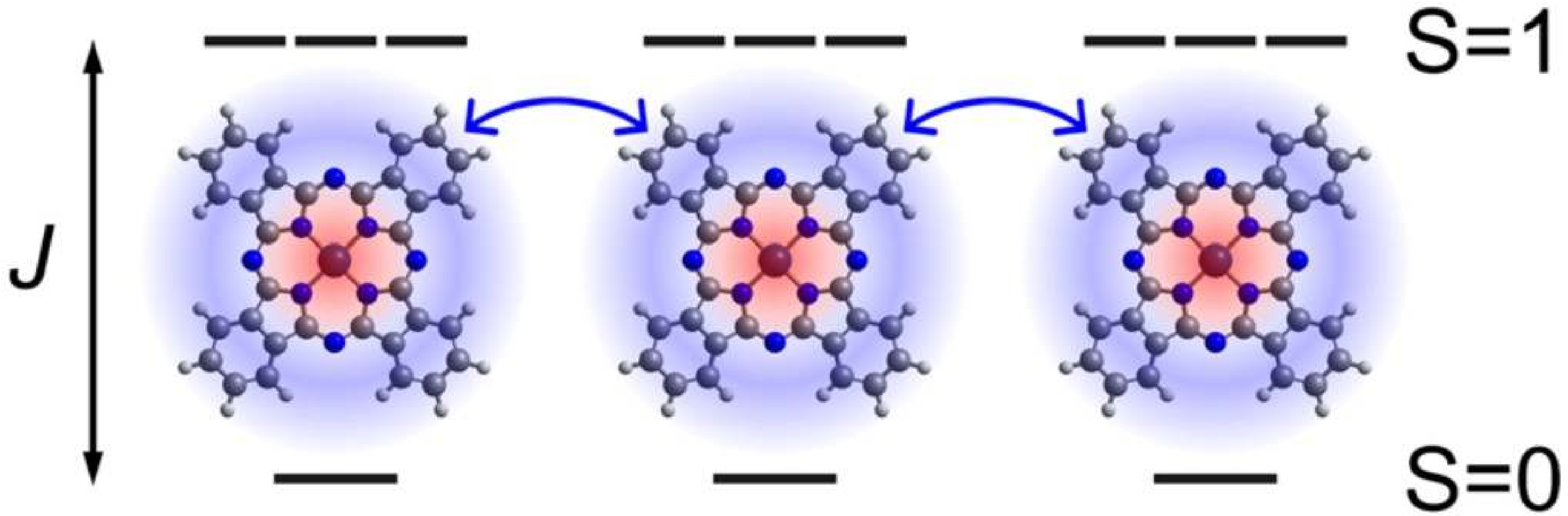
A triplet in the first molecule



Can jump to the second molecule

Exchange coupling between molecules leads to propagating triplon excitations

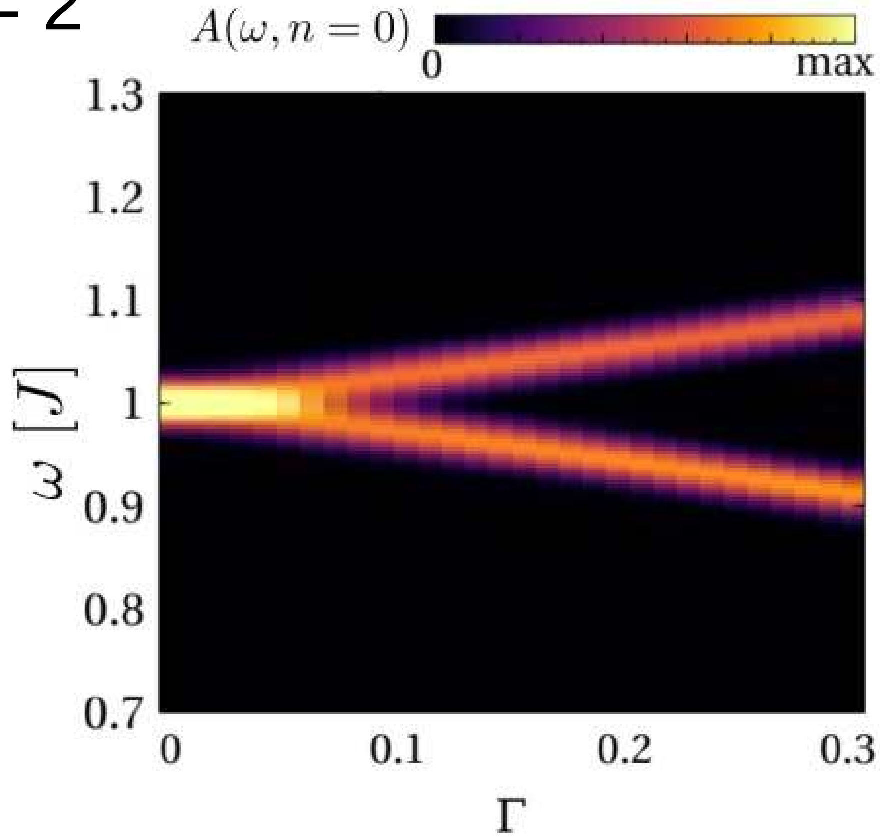
A chain of triplons



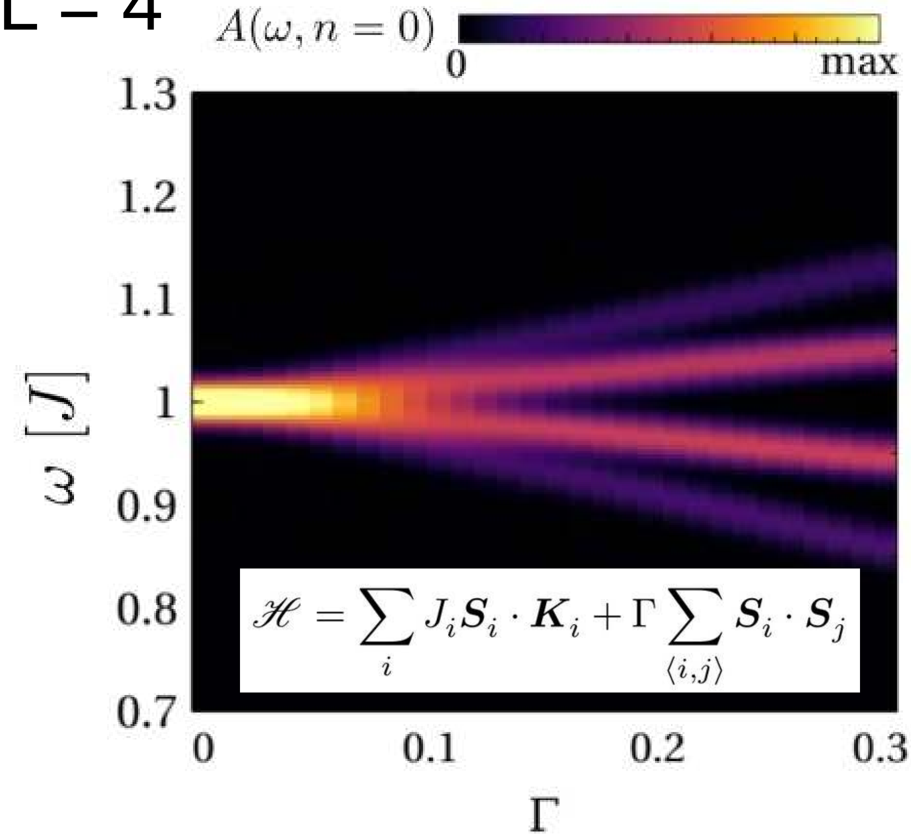
$$\mathscr{H} = \sum_i J_i \boldsymbol{S}_i \cdot \boldsymbol{K}_i + \Gamma \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

Chains of triplons

L = 2



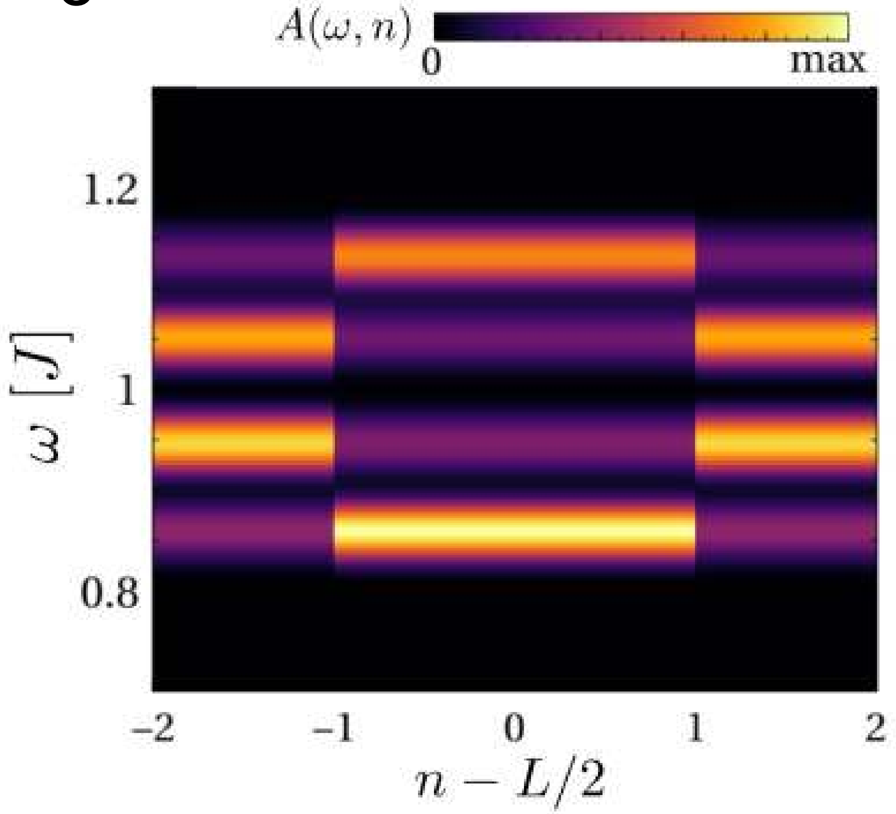
L = 4



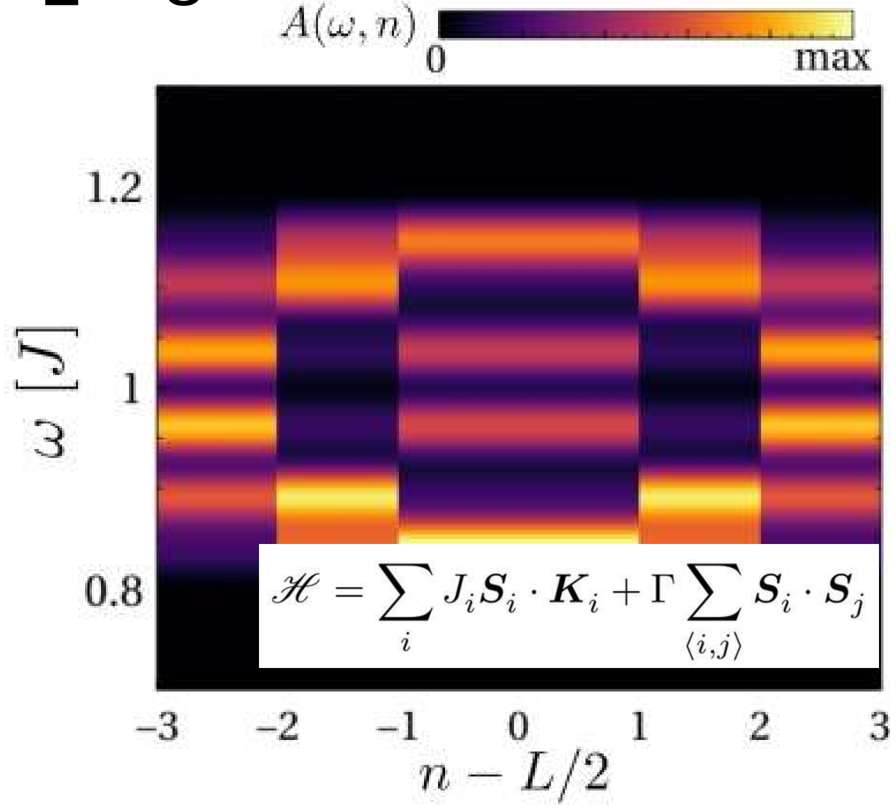
$$\mathscr{H} = \sum_i J_i \boldsymbol{S}_i \cdot \boldsymbol{K}_i + \Gamma \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

Chains of triplons

L = 6



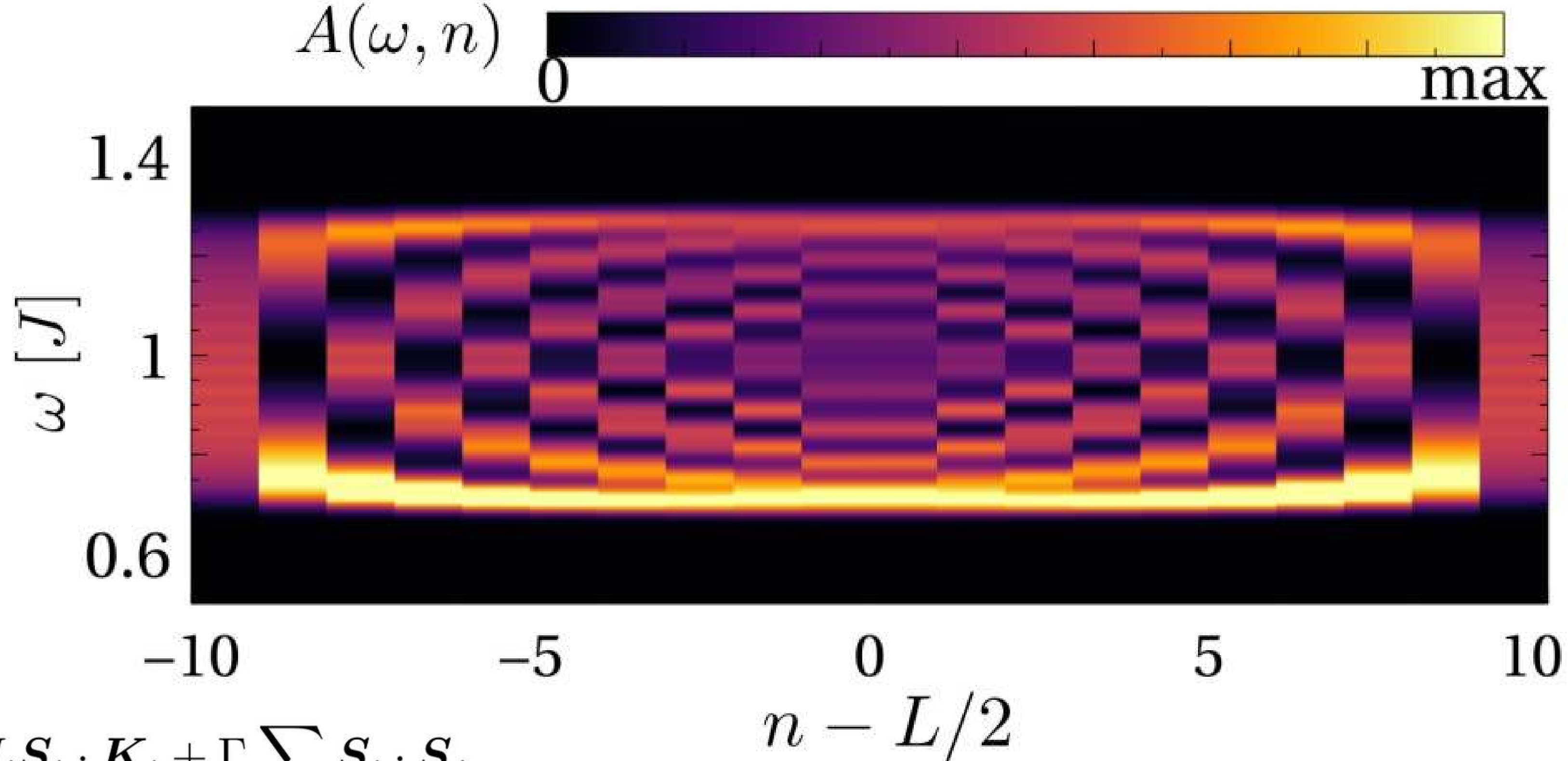
L = 8



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

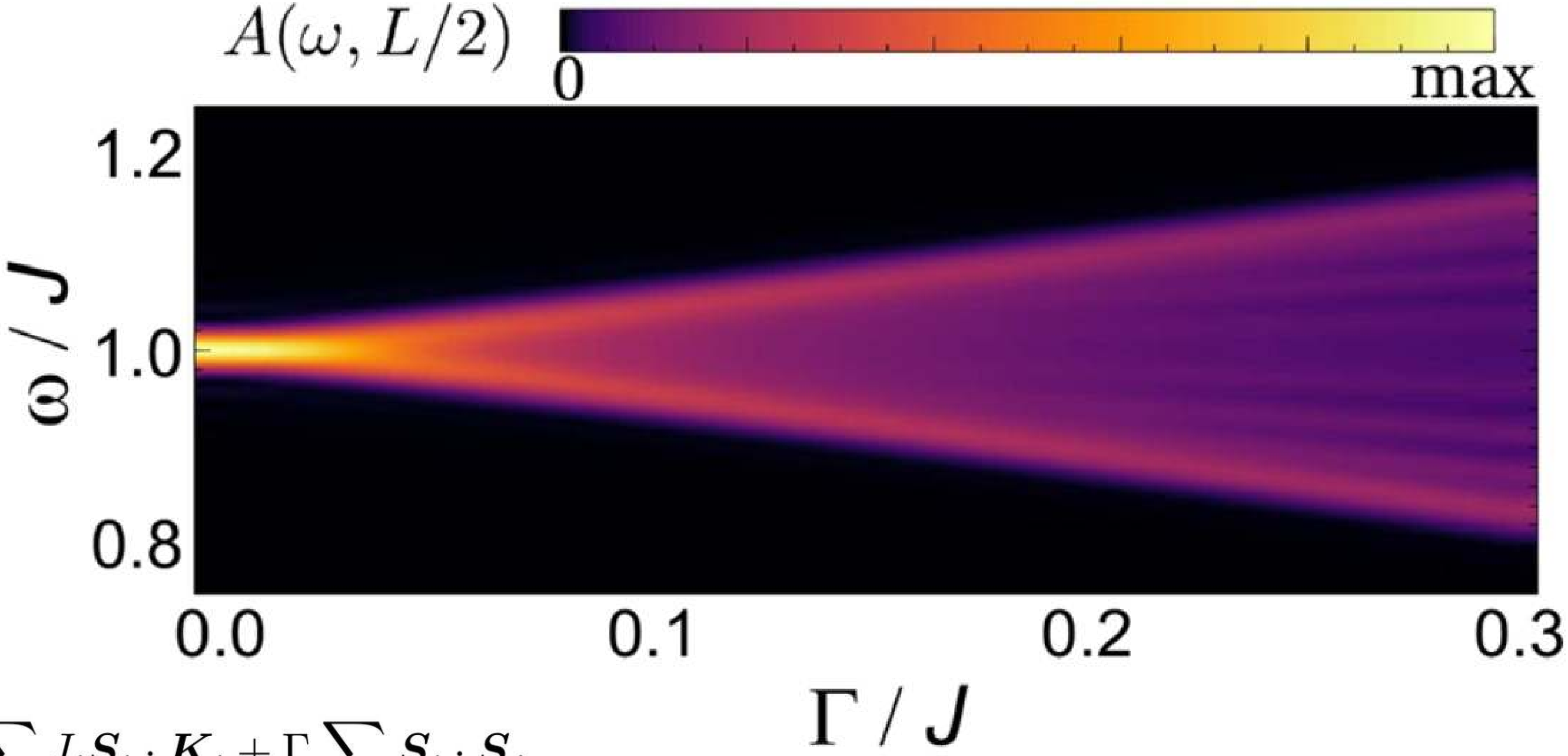
Chains of triplons

L = 20



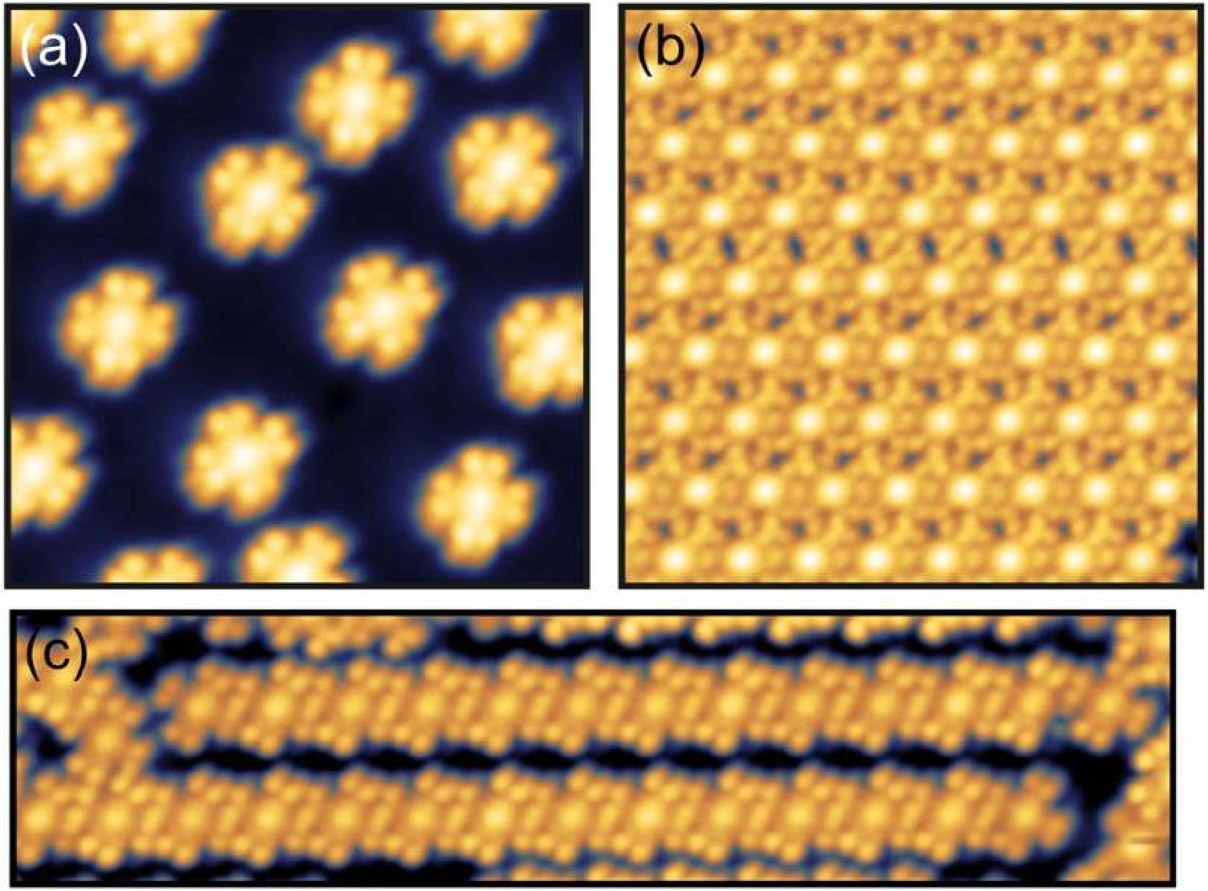
$$\mathcal{H} = \sum_i J_i \boldsymbol{S}_i \cdot \boldsymbol{K}_i + \Gamma \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

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

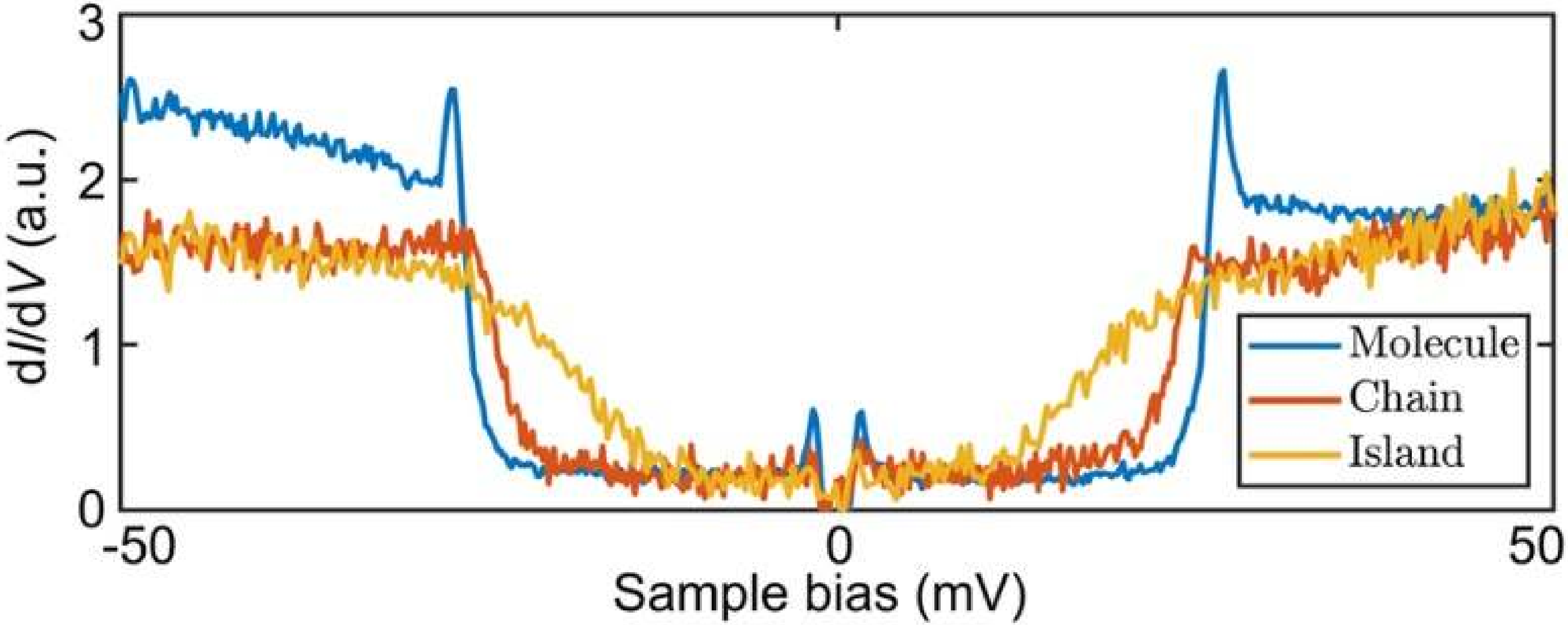


0D

2D

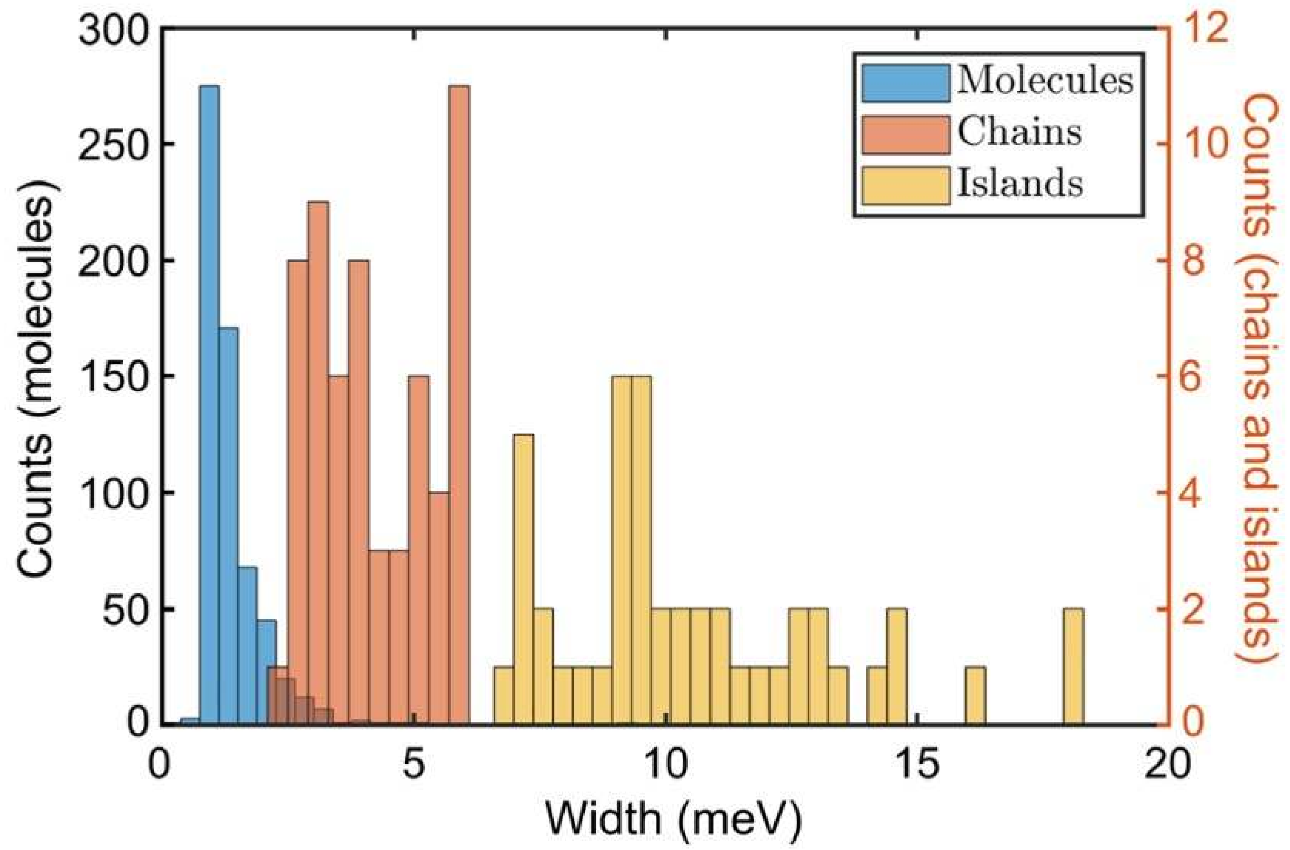
1D

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



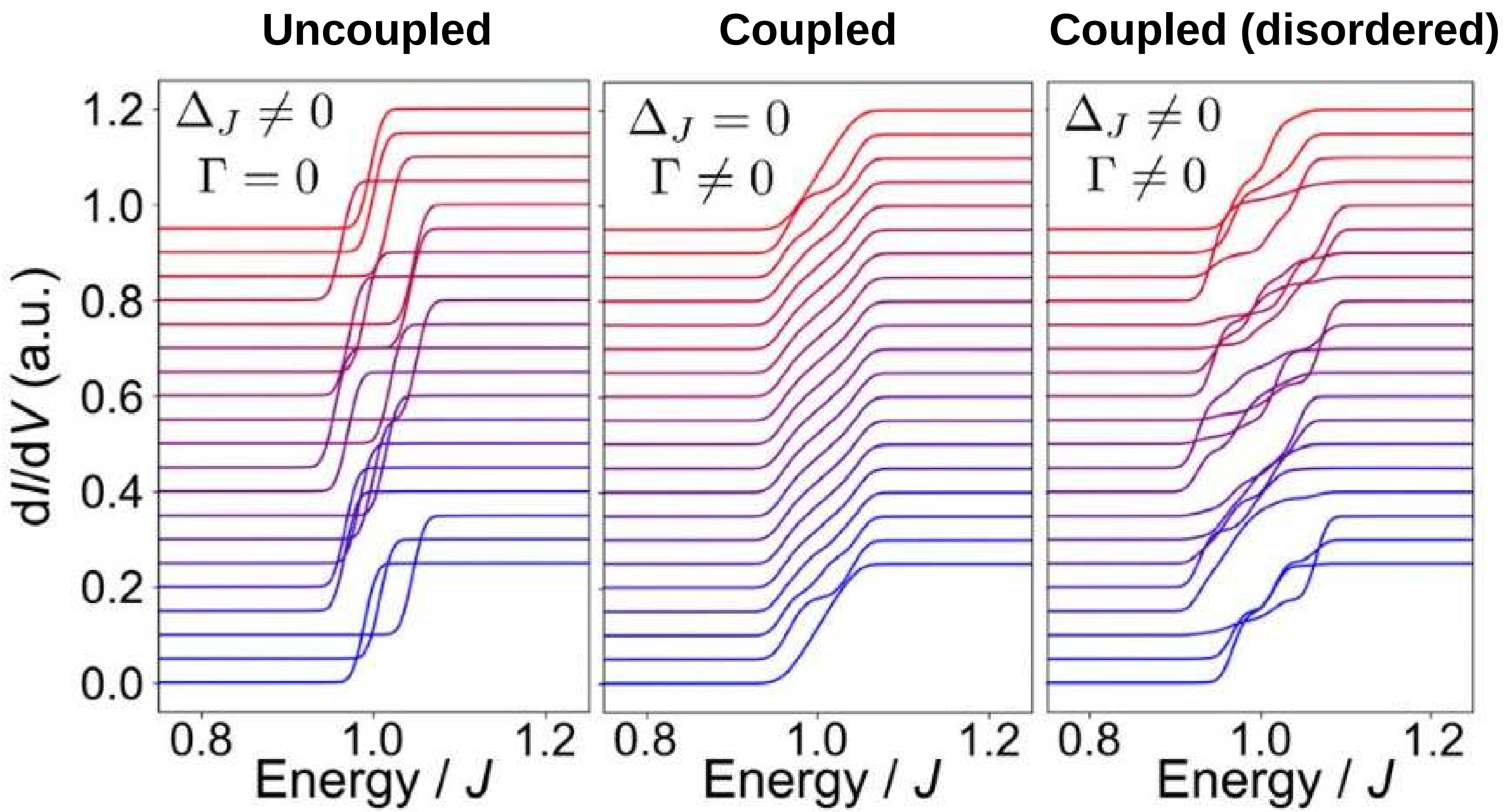
The width of the step is bigger for islands than for molecules

Statistic of the inelastic steps

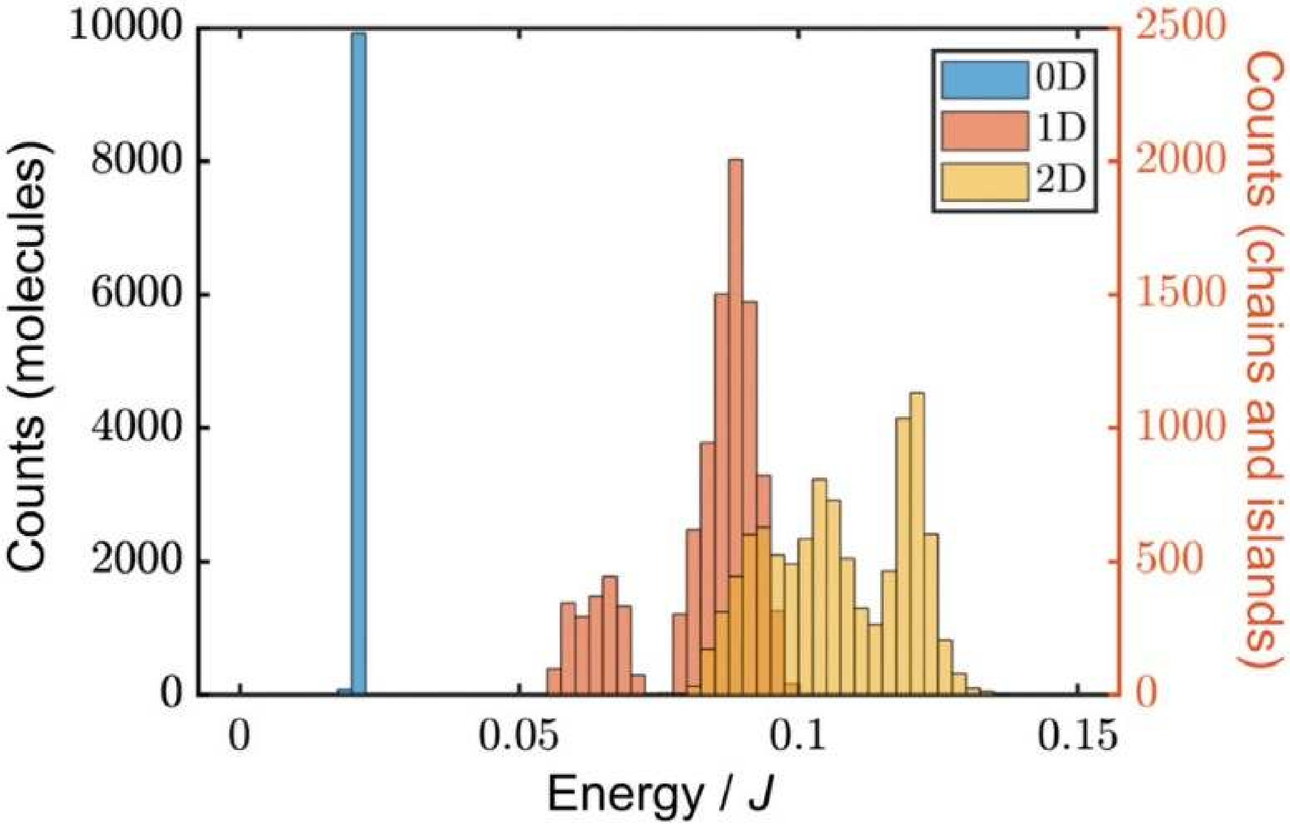


2D arrays have the largest width of the spin excitation

Coupled and uncoupled inelastic excitation

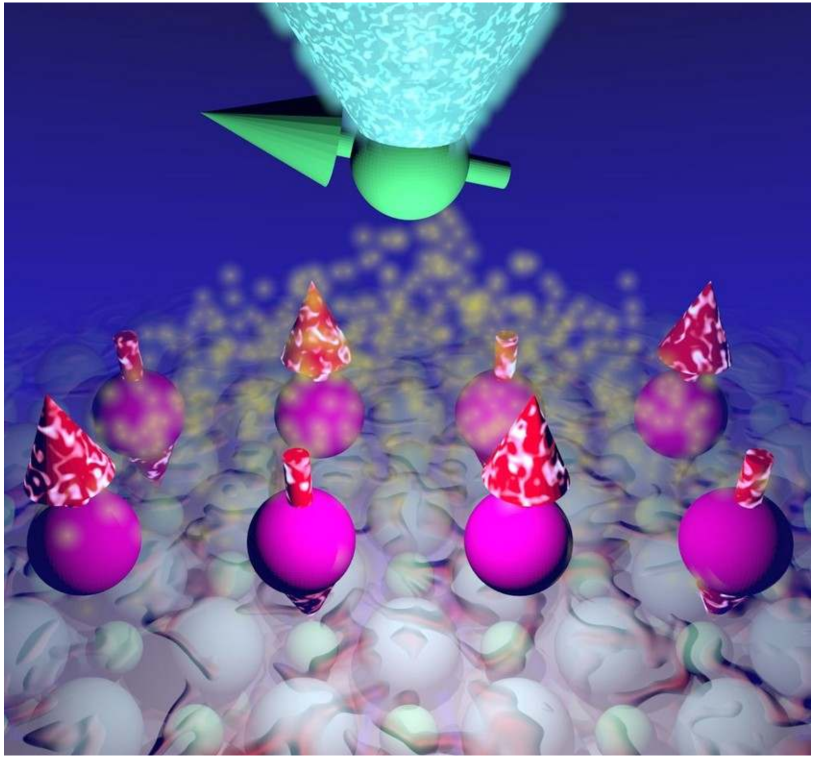


Statistics of the theoretical model



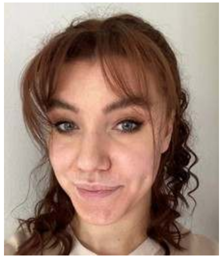
2D arrays have the largest width of the spin excitation

Hamiltonian learning nanoscale magnets



Hamiltonian learning nanoscale magnets

Netta Karjalainen



Zina Lippo

Rouven Koch

Guangze Chen

Adolfo Fumega

Phys. Rev. Applied 20, 024054 (2023)

The problem of Hamiltonian learning

How can we go from observables to the Hamiltonian?

Conventional workflow in theoretical physics

Solve the Hamiltonian — Compute an observable

$$H \longrightarrow \langle \Psi | O | \Psi \rangle$$

The problem we often find experimentally

Measure an observable — Determine its Hamiltonian

$$\langle \Psi | O | \Psi \rangle \longrightarrow H$$

How can we perform this task?

Can we use machine learning to solve problems in quantum matter?

Supervised learning

"Dog"

Labeled prediction

Generative learning

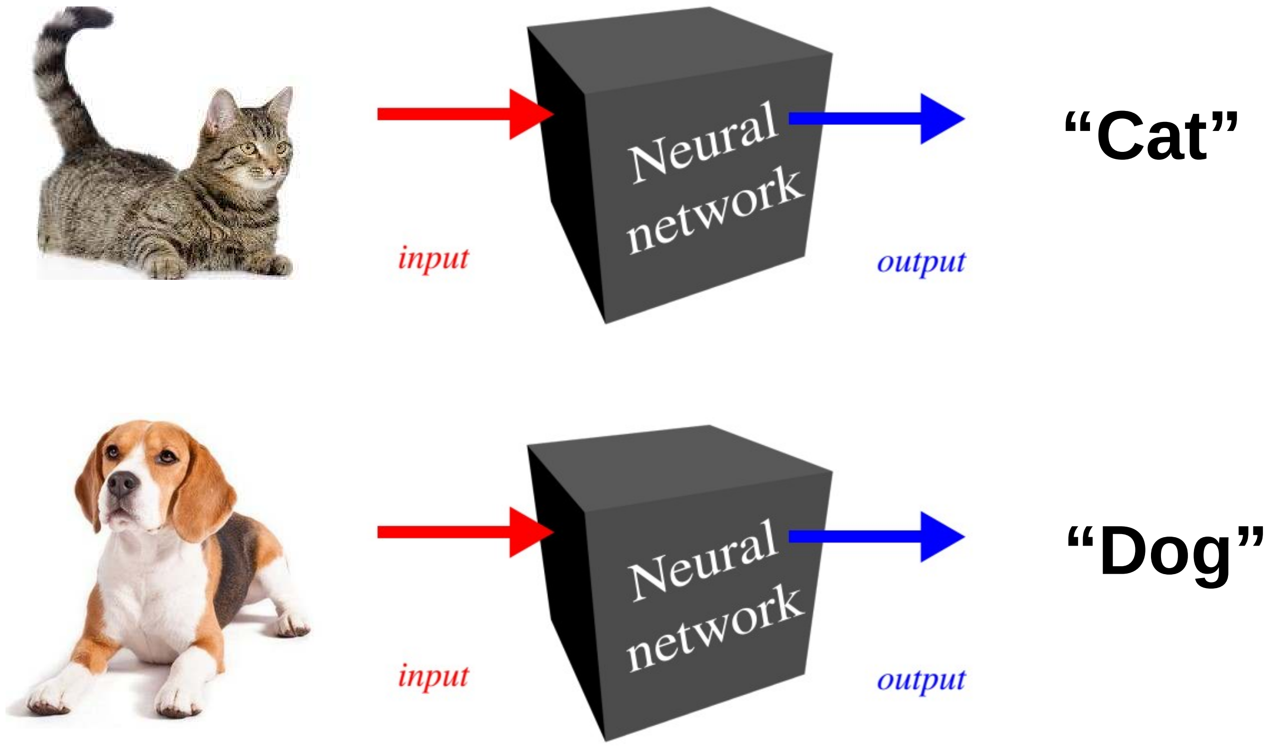
Probability Modeling

Reinforcement learning

Reward-based decision

(and others)

Machine learning in classification problems



Hamiltonian learning: combining theory and experiment

Train a machine learning algorithm with simulated data

so that the parameters of each Hamiltonian are explicitly know

$$H(\lambda_i^{\text{theo}}) \rightarrow \langle O \rangle_{\text{theo}} \rightarrow \boxed{\text{Neural network}} \rightarrow \lambda_i^{\text{theo}}$$

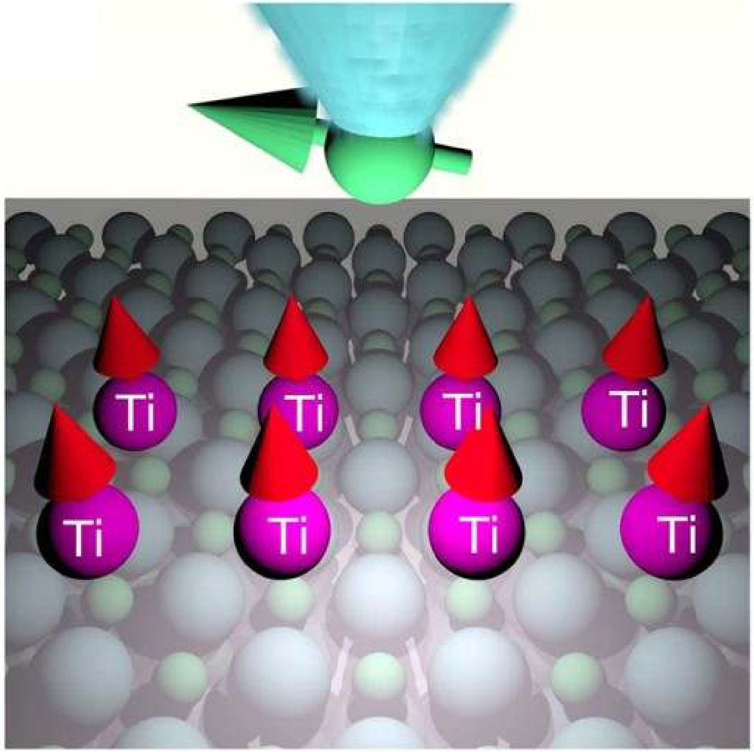
Hamiltonian

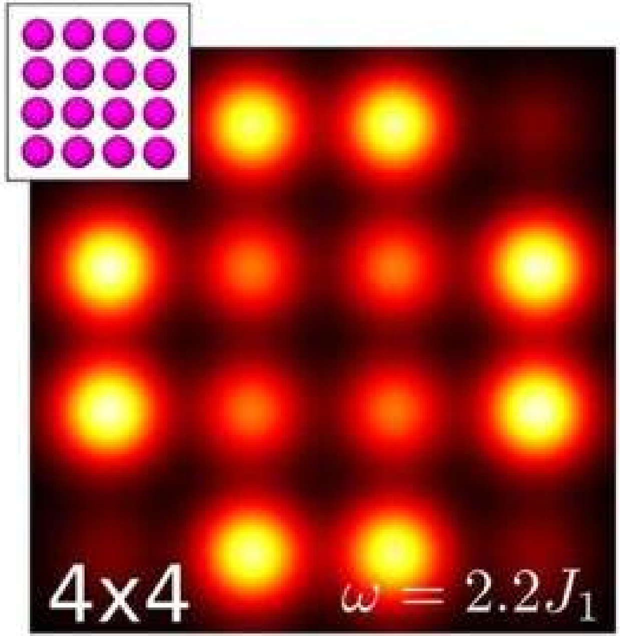
With the trained algorithm, evaluated in experimental data to extract the parameters

$$\langle O \rangle_{\exp} \rightarrow \boxed{\text{Neural network}} \rightarrow \lambda_i^{\exp}$$

Hamiltonian

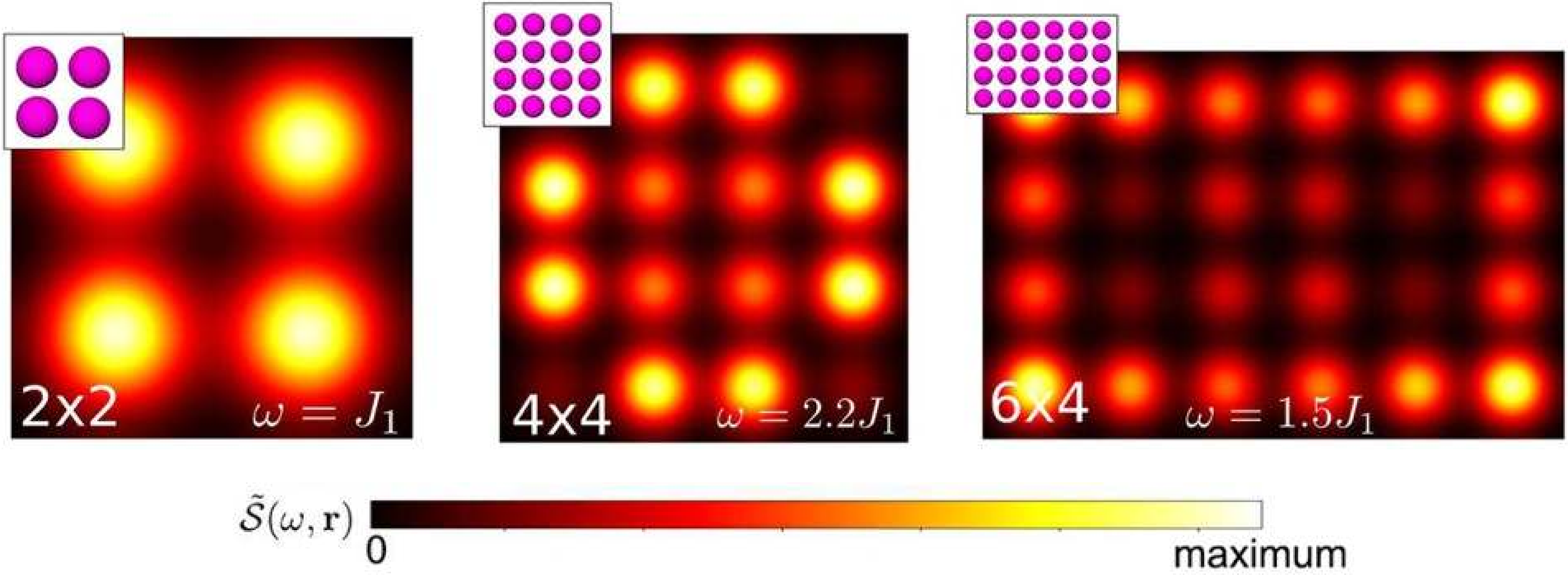
Spatially resolved excitations





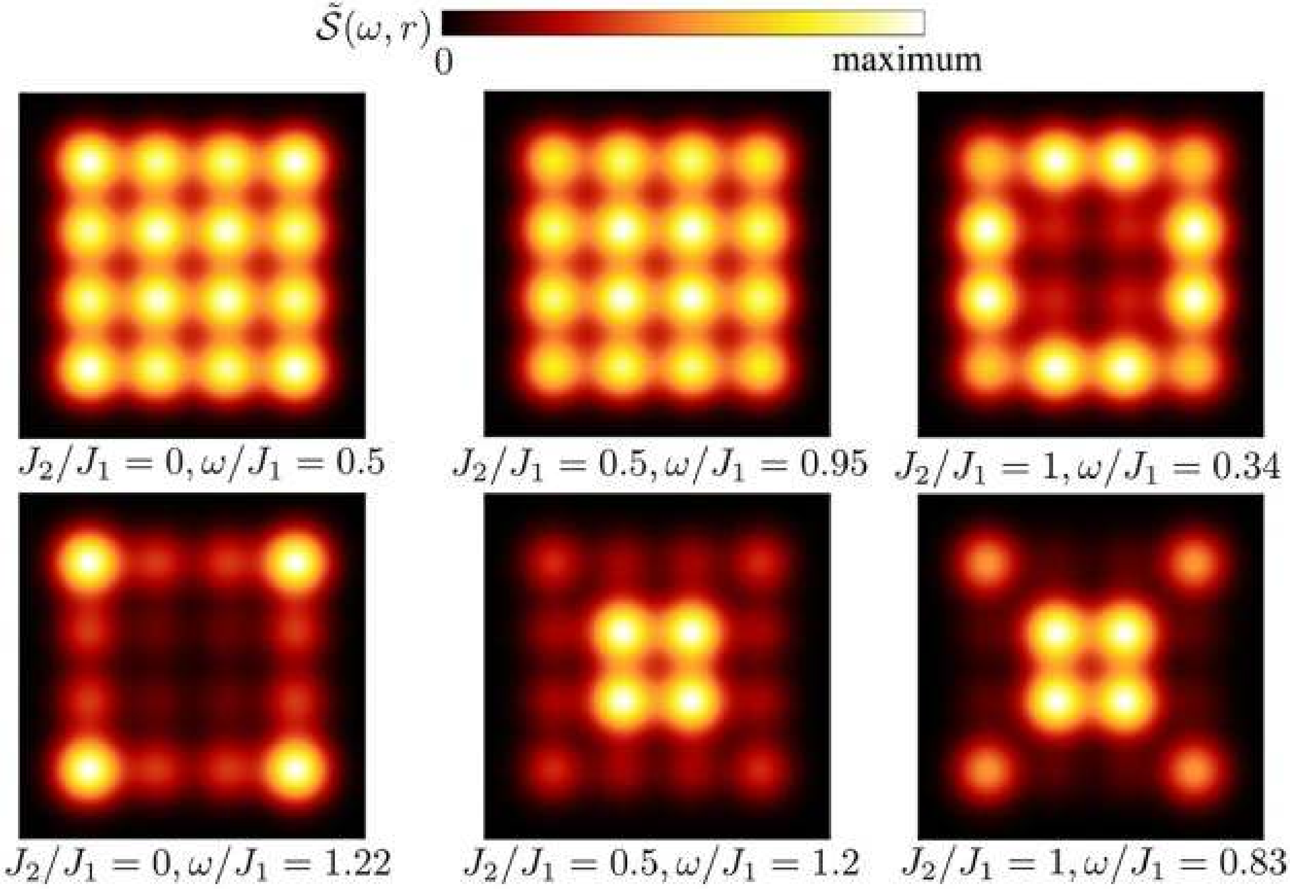
What can we learn from the Hamiltonian using real-space information?

Spatially resolved excitations



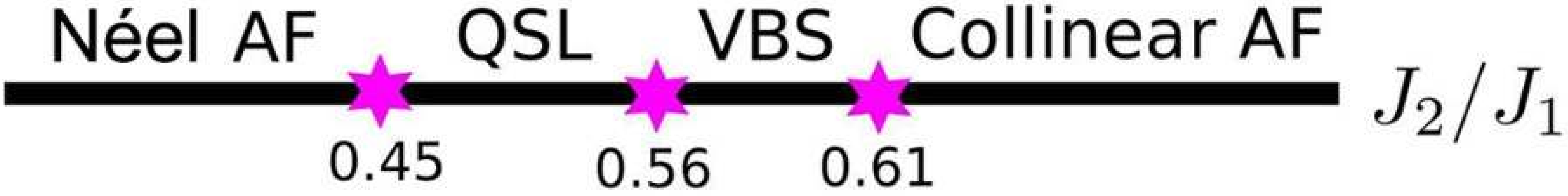
Spin excitations behave like particle in a box states

Spin excitation modes in spin islands



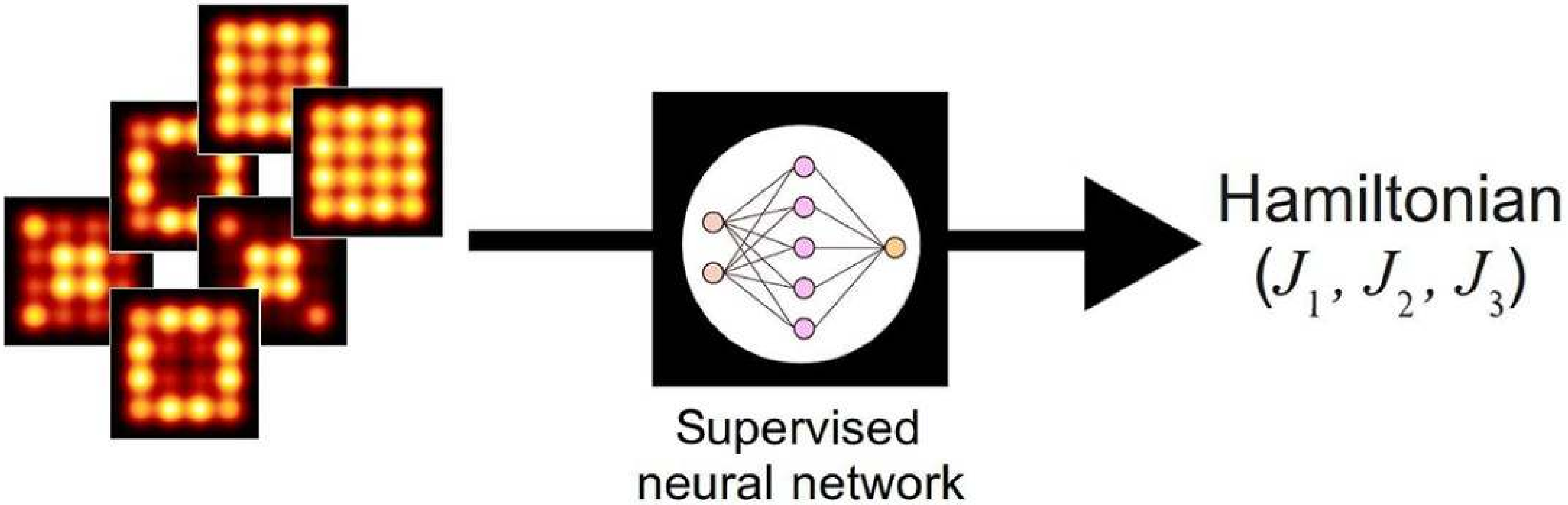
The extended Heisenberg model

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



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

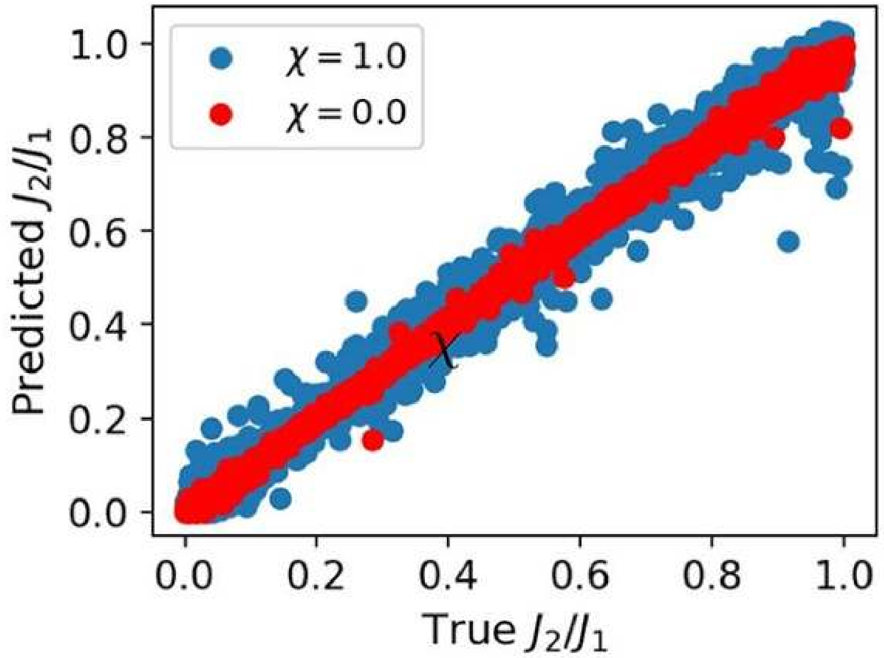
The idea of Hamiltonian learning

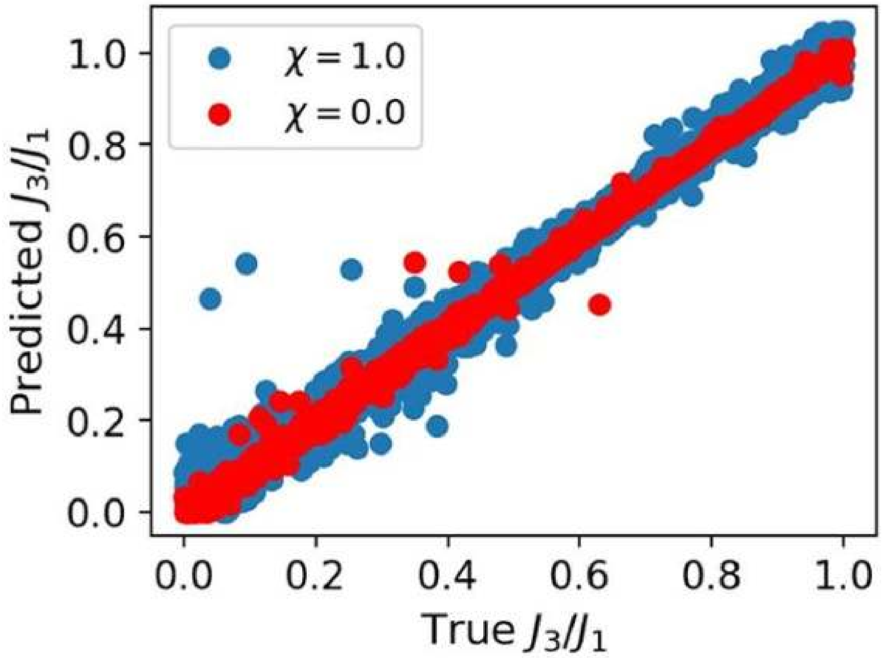


Provide the spectroscopy as input, obtain the Hamiltonian as output

Real VS predicted exchange parameters

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

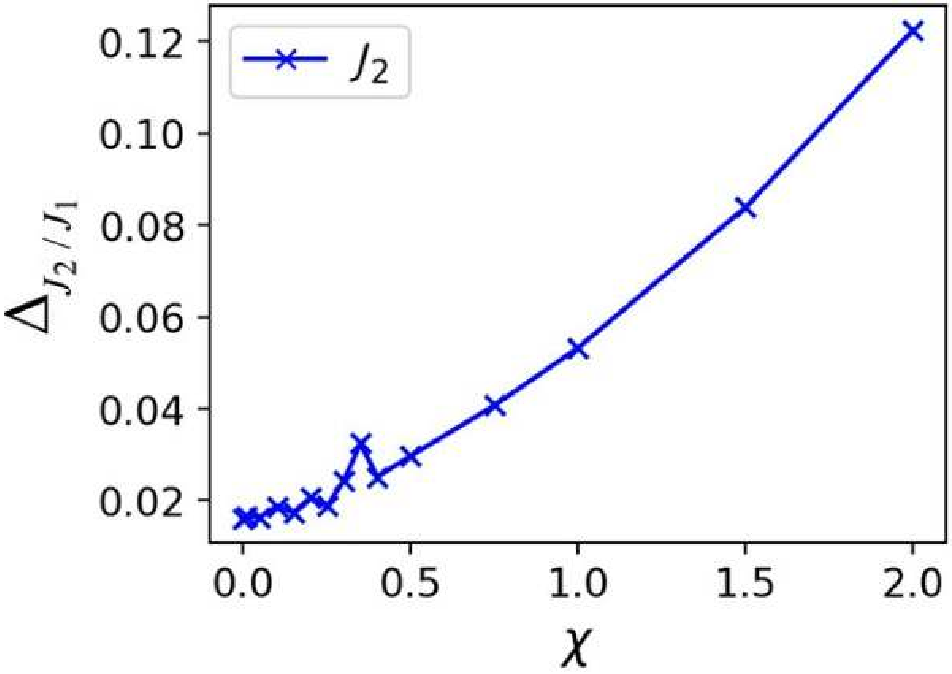


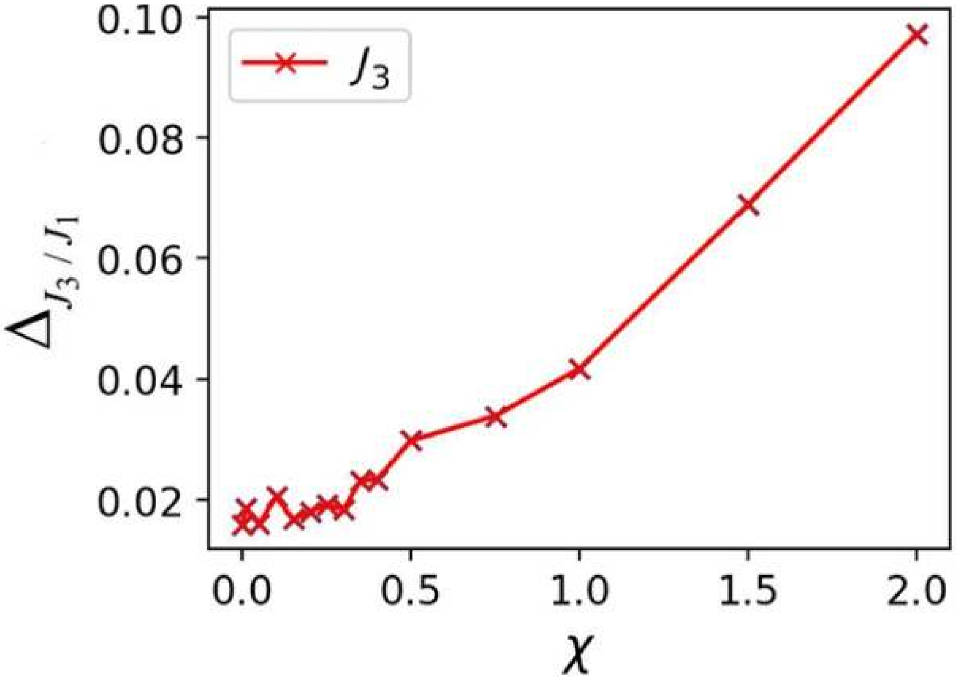


A supervised learning algorithm extracts faithfully the exchange parameters

Predictions with noise

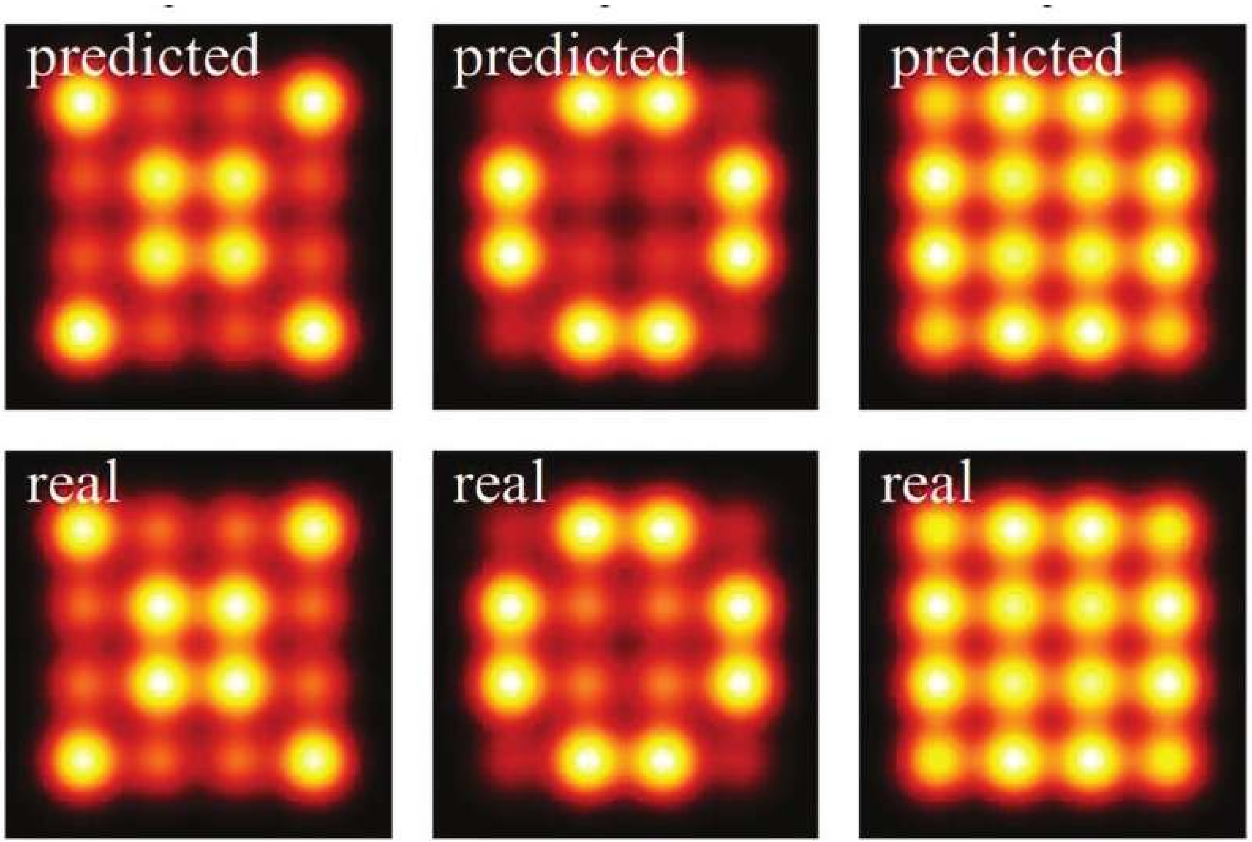
$$\mathcal{S}(\omega, \mathbf{r}_i)_{\text{noisy}} = \mathcal{S}(\omega, \mathbf{r}_i) \cdot |1 + \zeta(\omega)| \qquad \zeta(\omega) \in [-\chi, \chi]$$



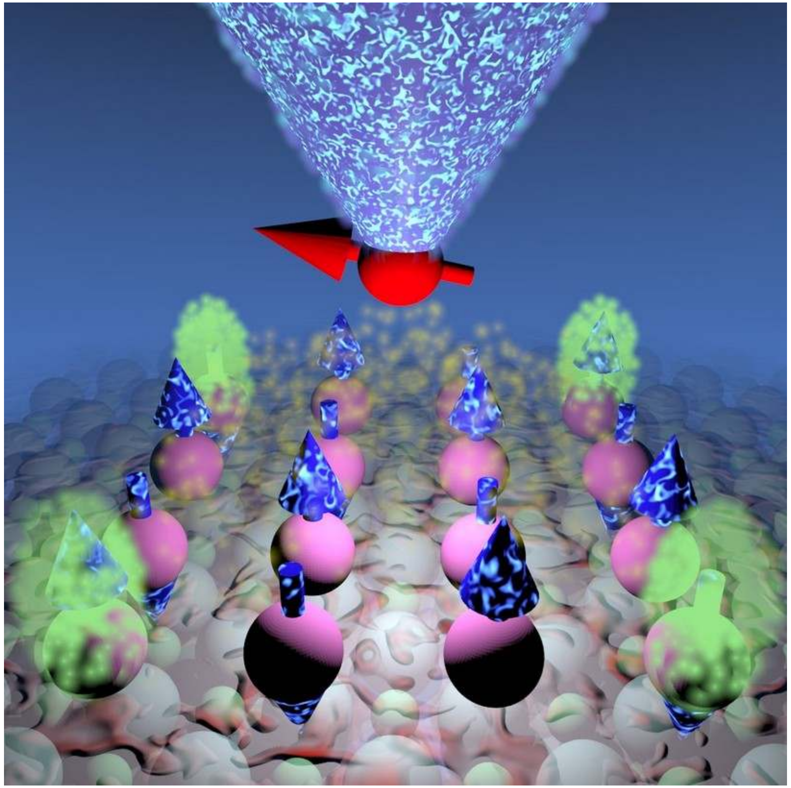


Quality of prediction remain good with sizable noise levels

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

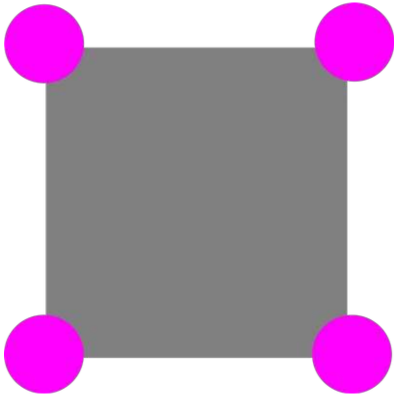
Topological quantum magnets

First order topological quantum magnet

1D gaped bulk
0D fractional edge modes

Nature 598, 287–292 (2021)

Second order topological quantum magnet



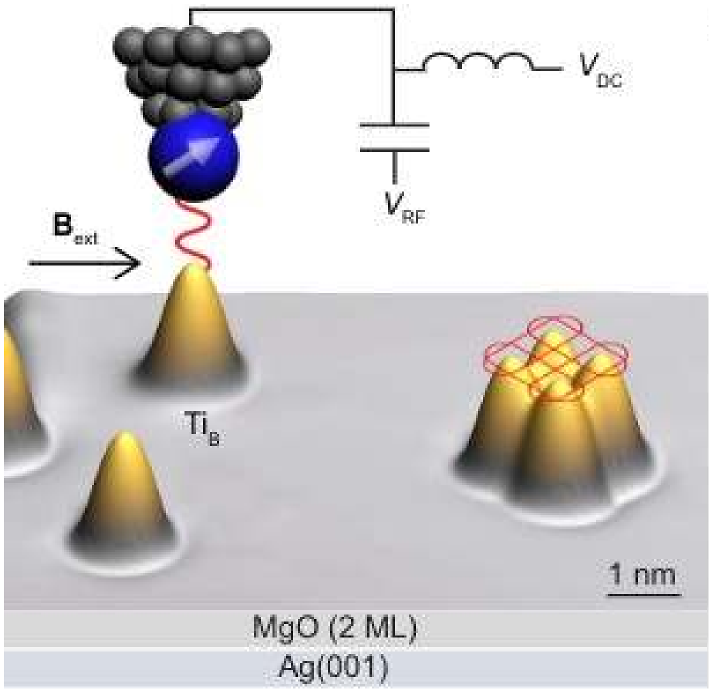
2D gaped bulk
0D fractional edge modes

Nature Nanotechnology (2024)

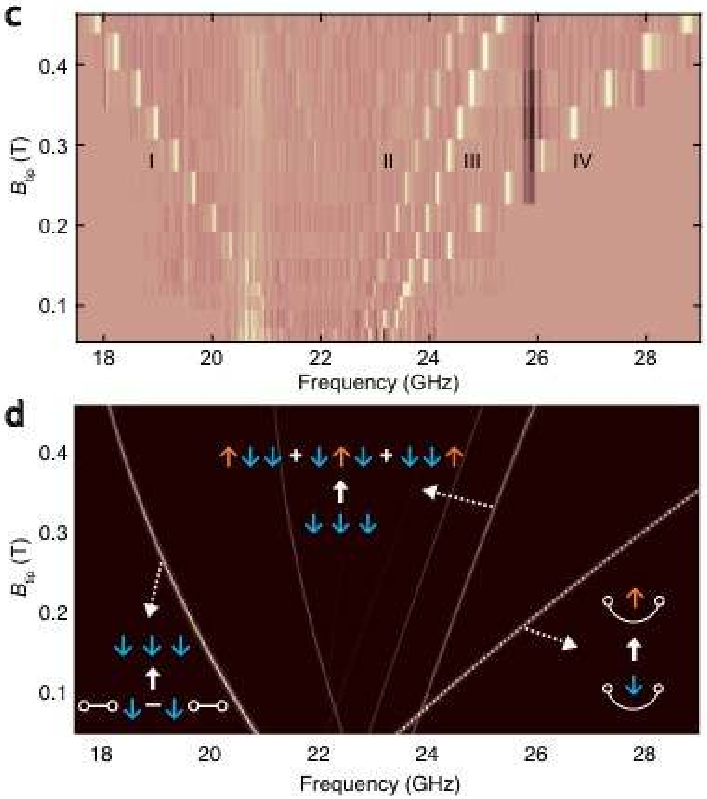
10.1038/s41565-024-01775-2

Artificial spin models with Ti@MgO

Ti@MgO (2x2 lattice)

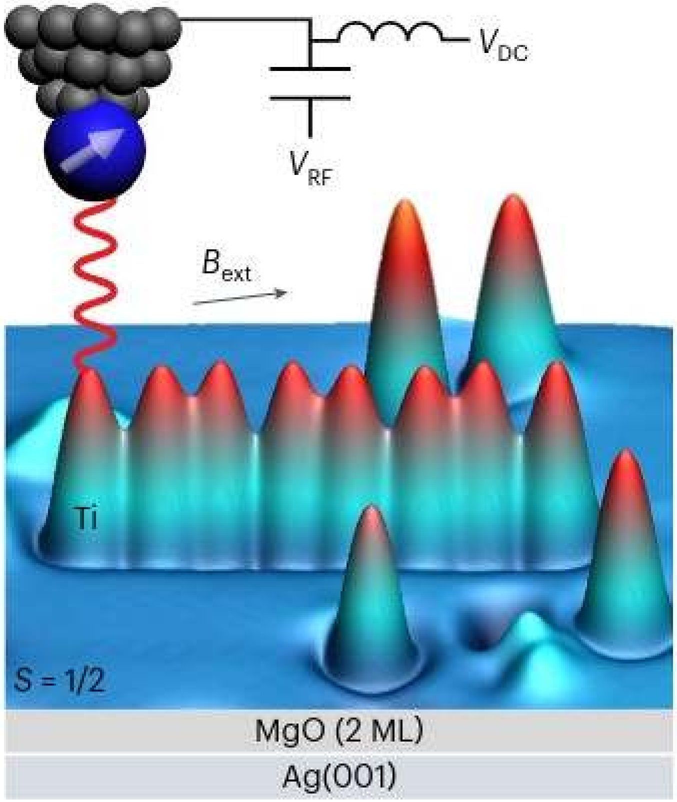


Nature Communications 12, 993 (2021)

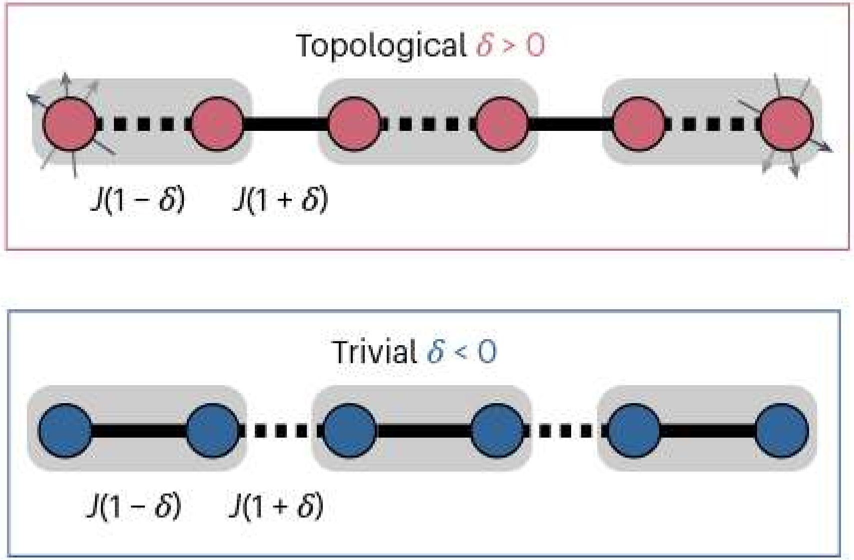


Can we create new states of matter?

First order topological quantum magnets



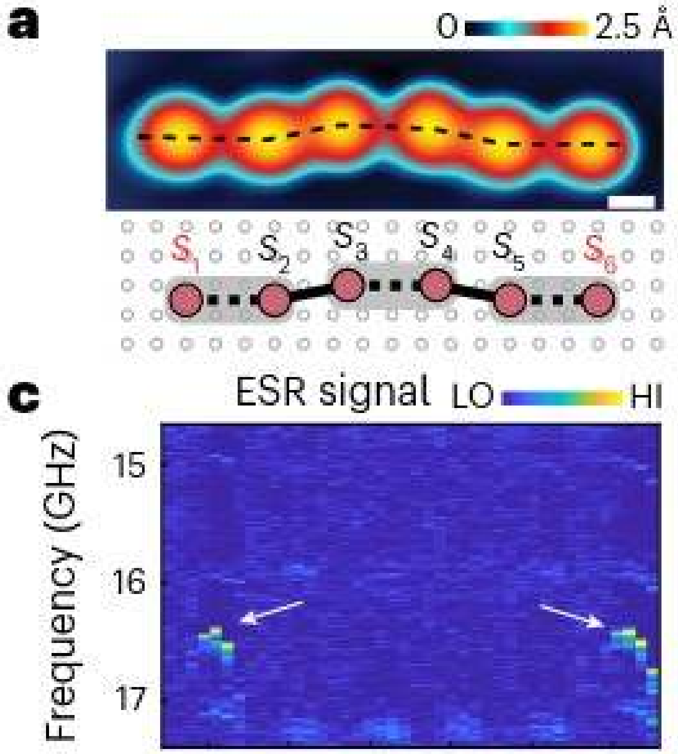
Two possible configurations



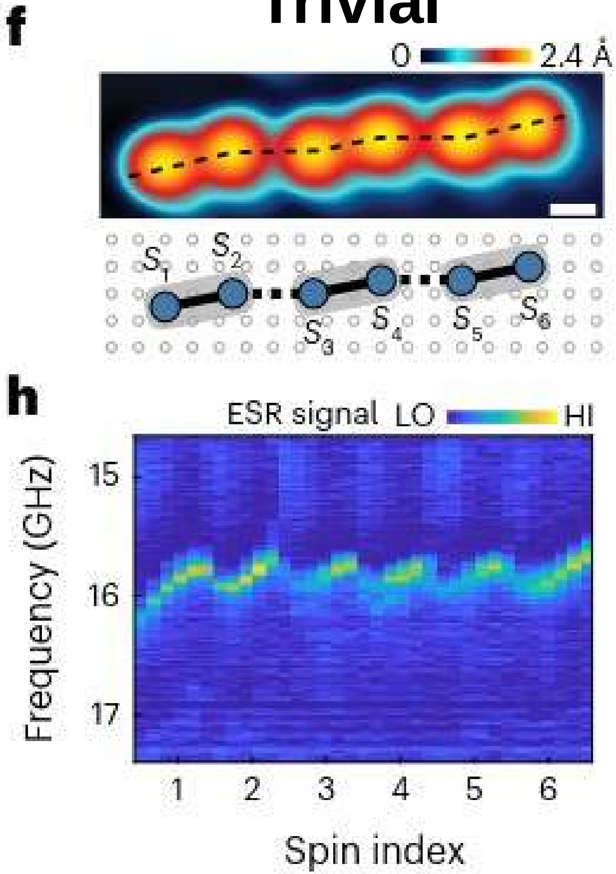
Nature Nanotechnology (2024)
10.1038/s41565-024-01775-2

First order topological quantum magnets

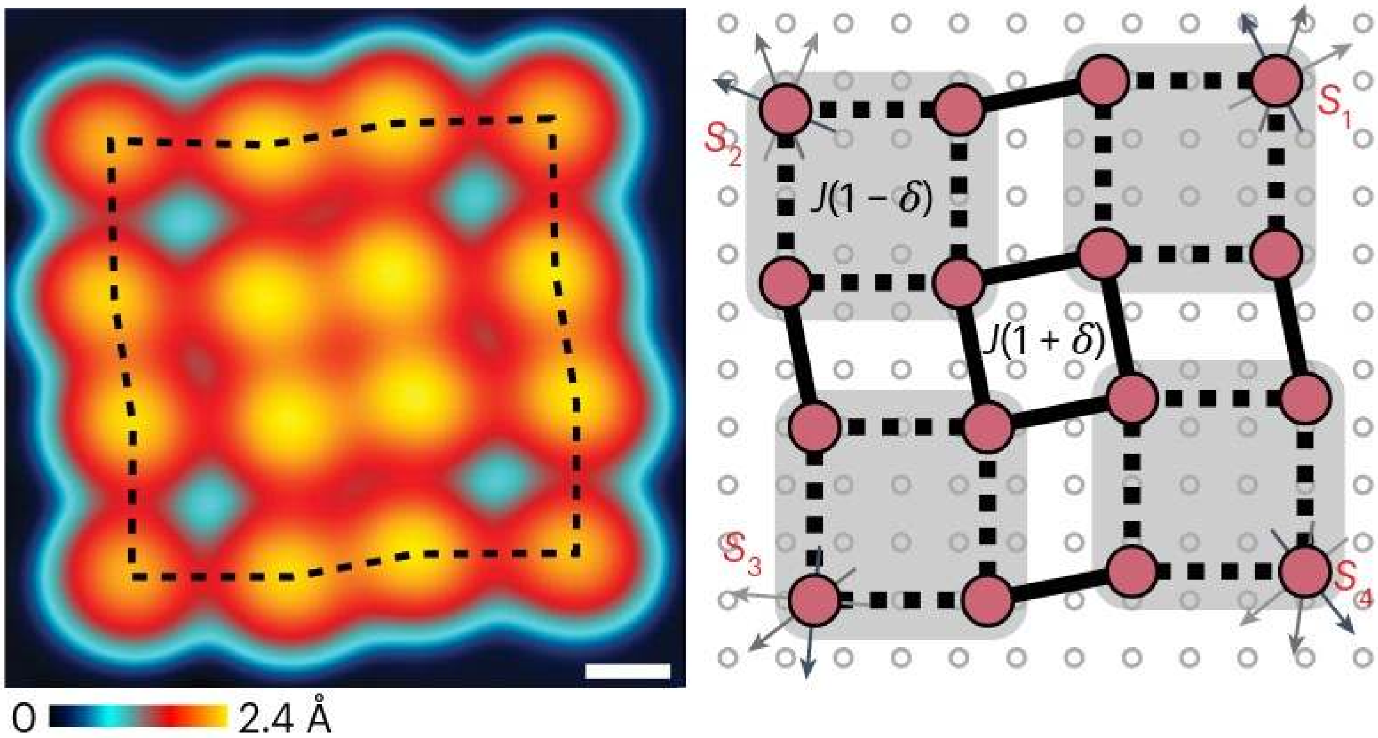
Topological



Trivial

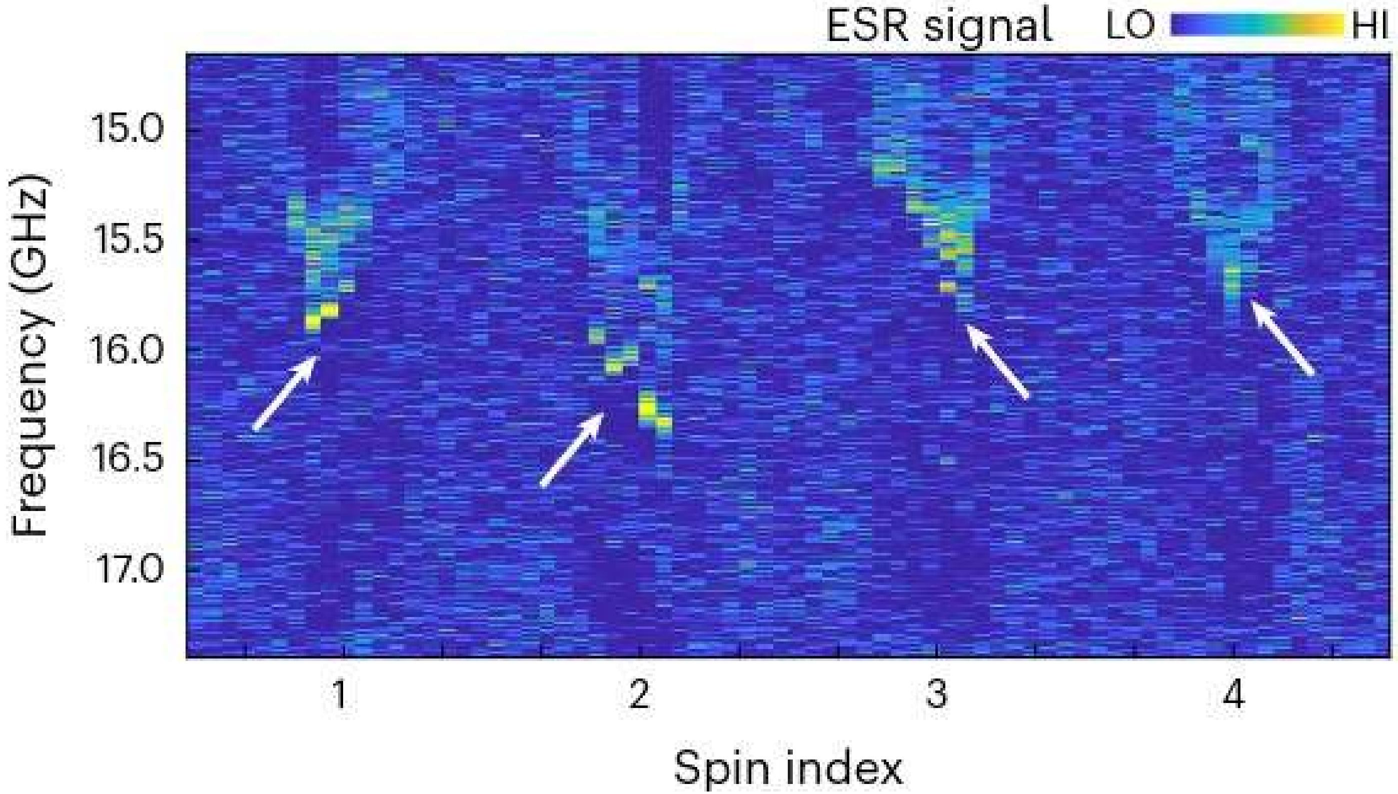


A higher order topological quantum magnet



The higher order topological quantum magnet shows topological corner modes

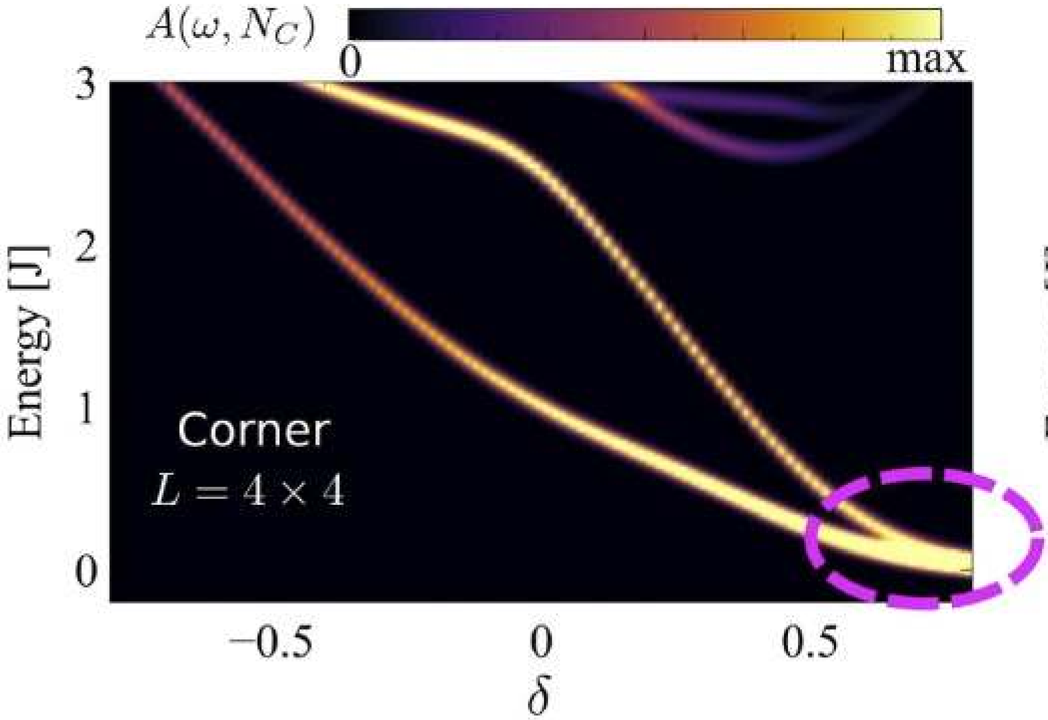
A higher order topological quantum magnet



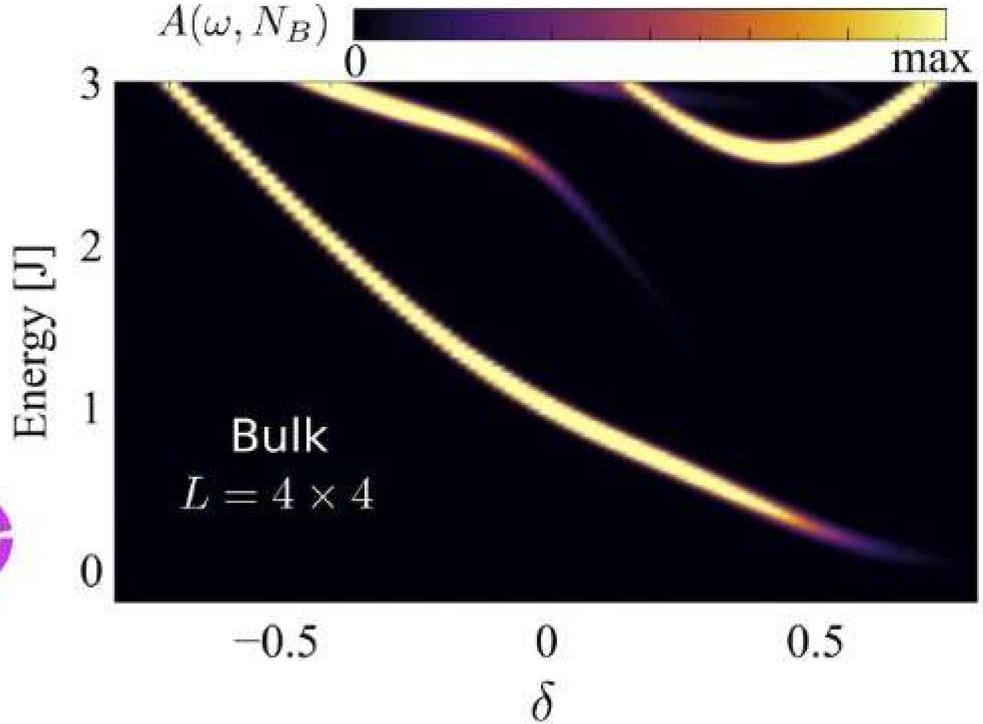
Topological corner modes are measured coexisting with a bulk spectral gap

A higher order topological quantum magnet

Corner spin excitations

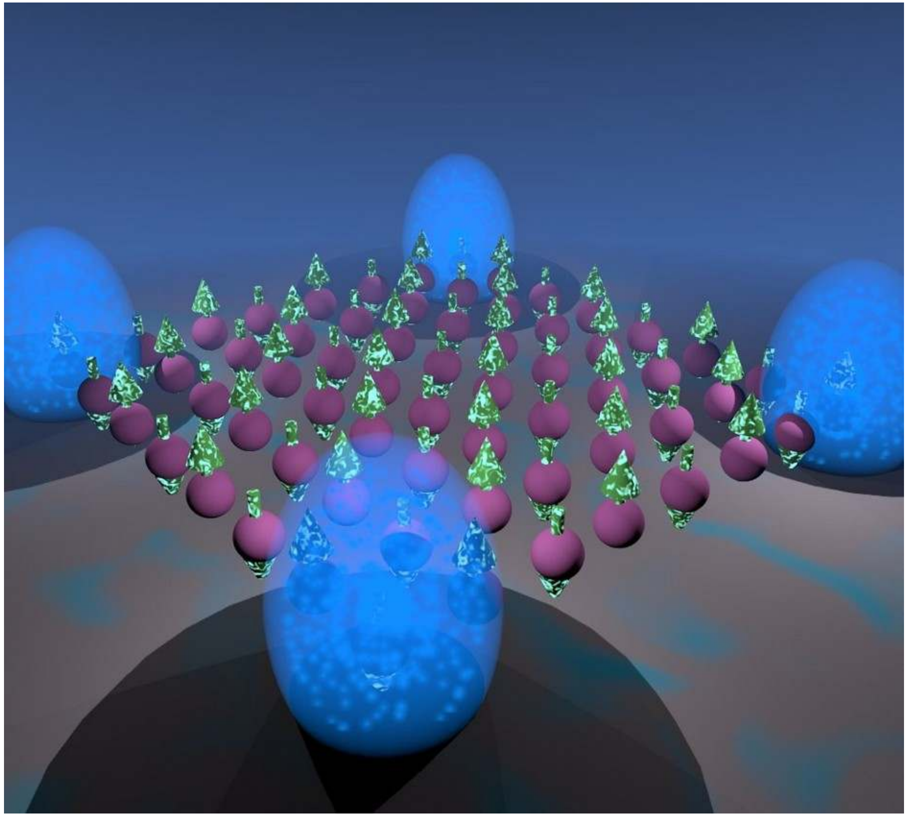


Bulk spin excitations

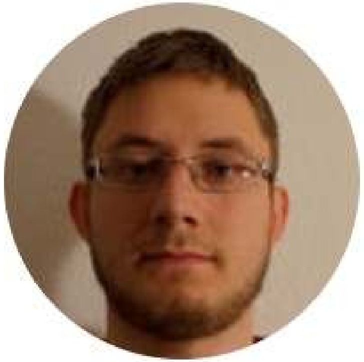


The tetramerization of the lattice creates topological corner spin excitations

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

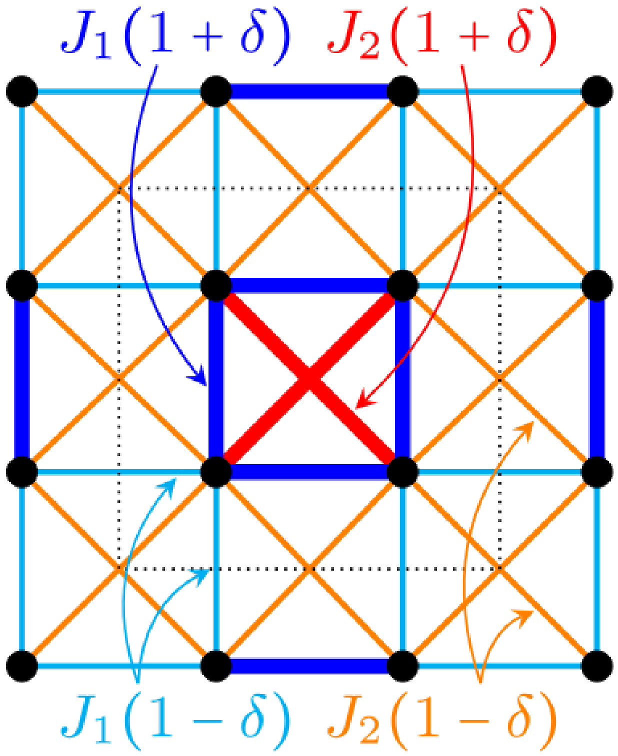


Pascal Vecsei

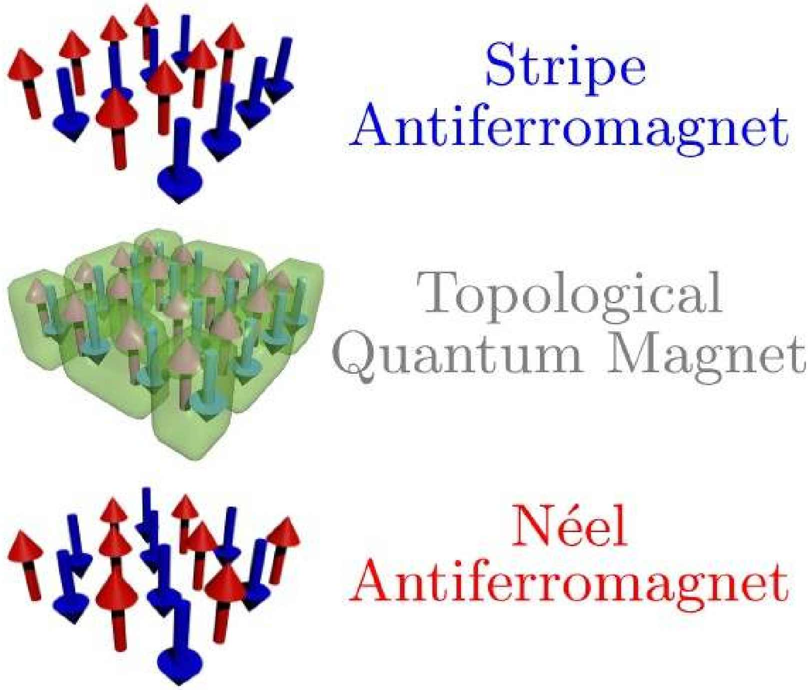


arXiv:2408.16453 (2024)

The model of a frustrated topological quantum magnet



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

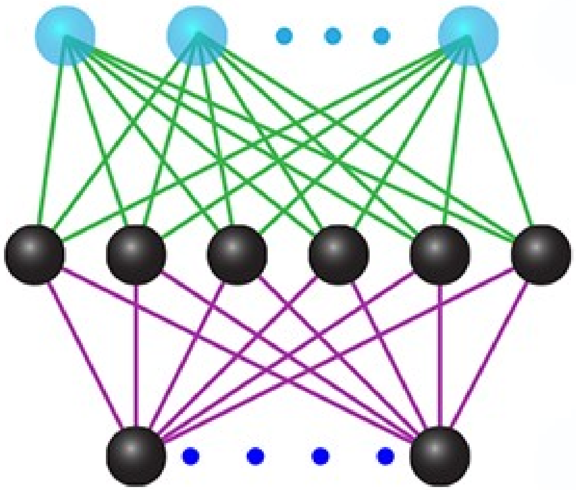


Solving frustrated quantum 2D models

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

Tensor-networks

For this wavefunction $|\Psi\rangle = \sum c_{s_1,s_2,...,s_L} |s_1, s_2, ...s_L\rangle$

A matrix product state takes a variational parametrization of the many-body wavefunction as

$$c_{s_1,s_2,....,s_L} = M_1^{s_1} M_2^{s_2} ....M_L^{s_3}$$

dimension 2^L

dimension $\sim Lm^2$

The ground state is obtained by minimizing

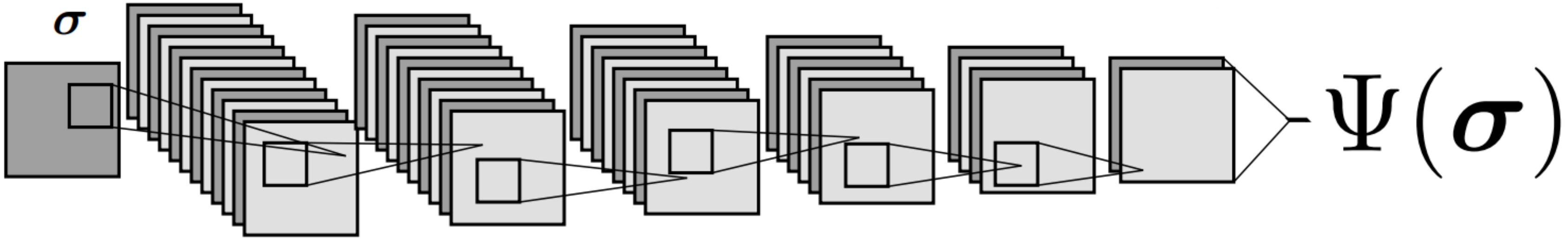
$$E = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} \qquad \frac{\delta E}{\delta M} = 0$$

Neural-network quantum states

Use machine leanring neural network architecture to encode the many-body wavefunction

$$c_{s_1, s_2, \ldots, s_L} = f(s_1, s_2, \ldots, s_L)$$

Deep neural network



$$|\Psi\rangle = \sum c_{s_1, s_2, \ldots, s_L} |s_1, s_2, \ldots s_L\rangle$$

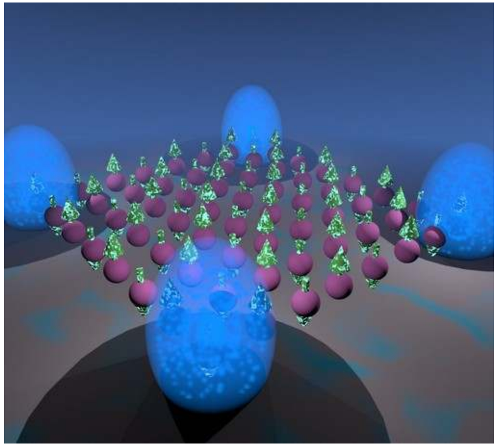
$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

The fundamental idea of tensor-networks and neural network quantum states

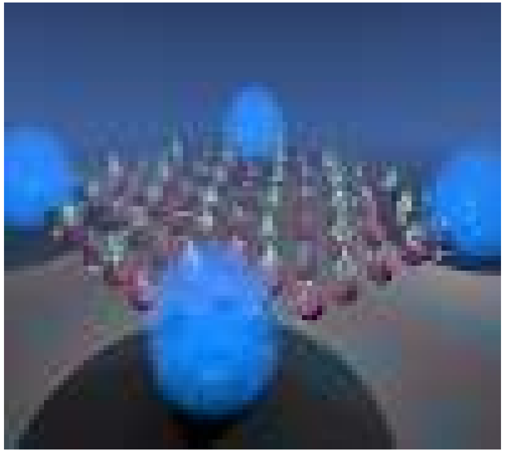
A many-body wavefunction a is a very high dimensional object

$$|\Psi\rangle = \sum c_{s_1,s_2,\ldots,s_L} |s_1, s_2, \ldots s_L\rangle$$

These methods allow “compressing” all that information in a very efficient way



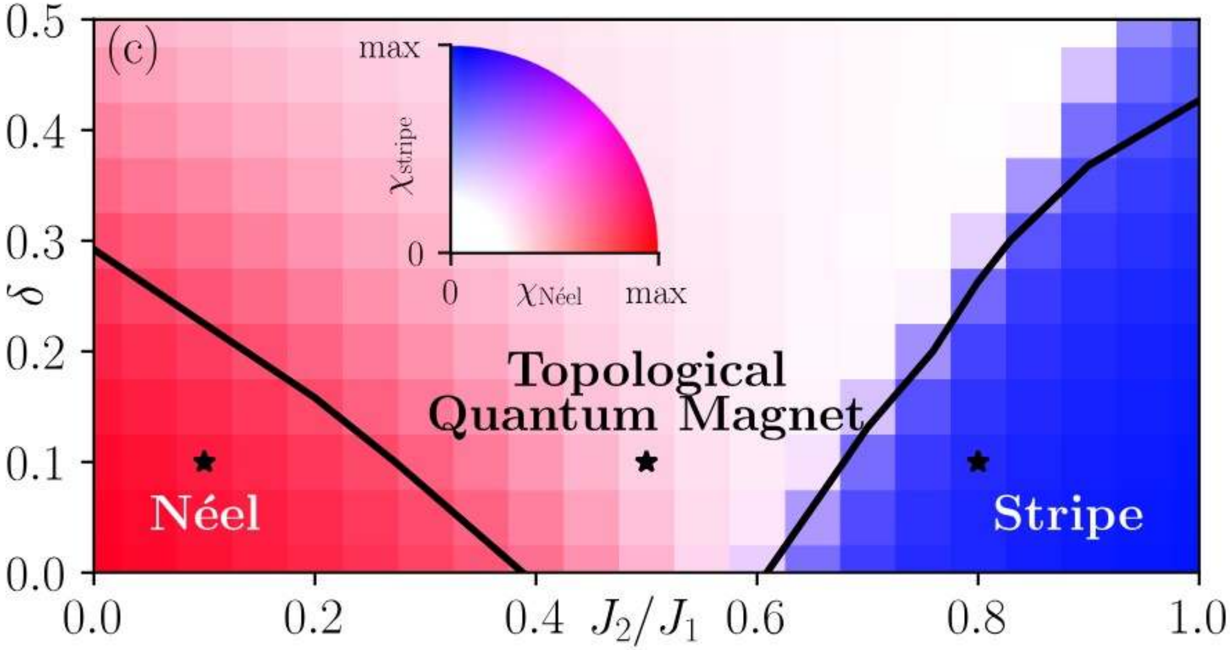
“True wavefunction”

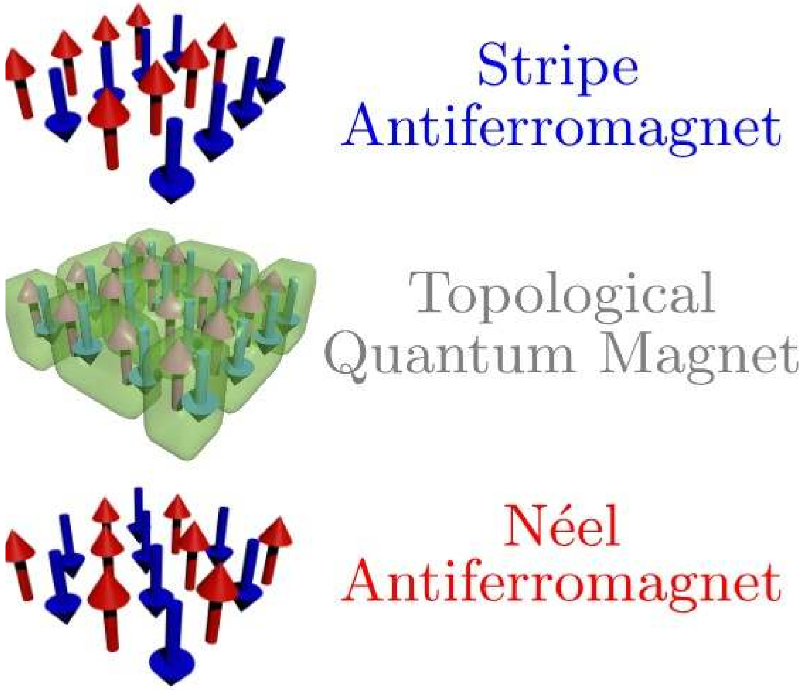


“Tensor-network/neural-network wavefunction”

The phase diagram of the higher order topological quantum magnet

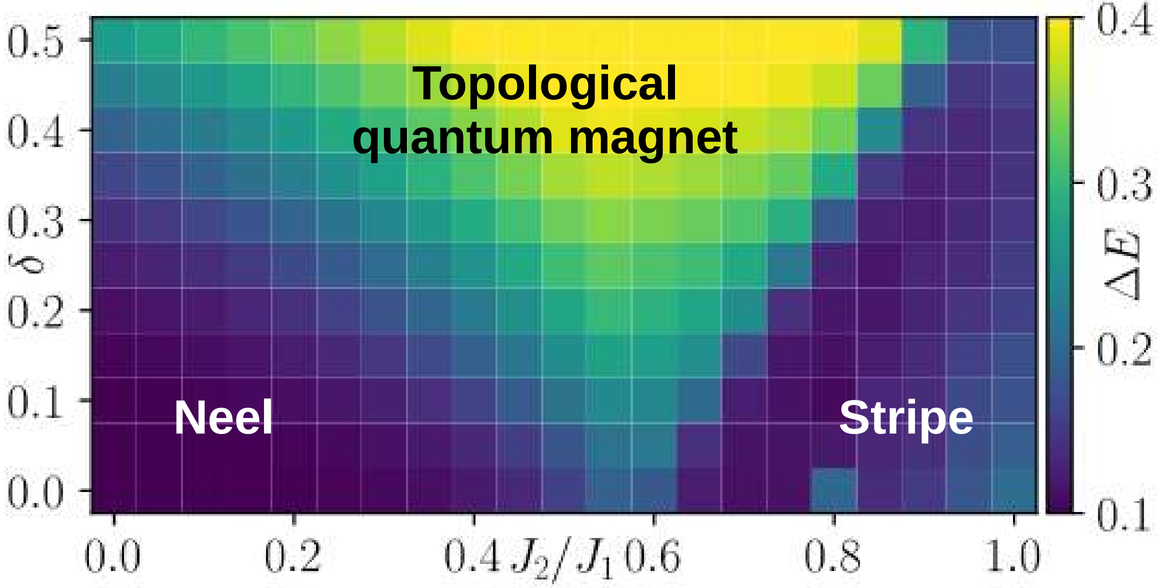
Phase diagram from susceptibilities

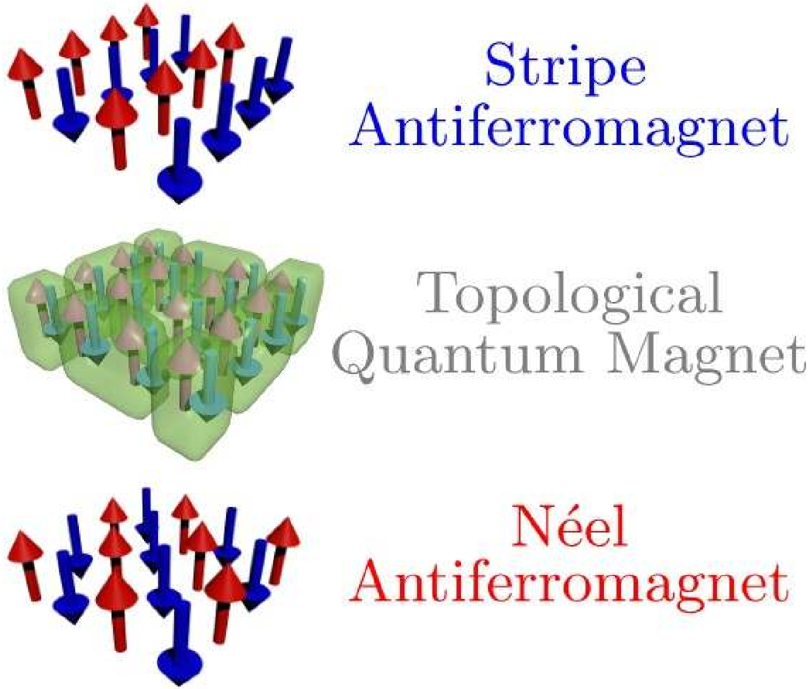




The phase diagram of the higher order topological quantum magnet

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

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

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

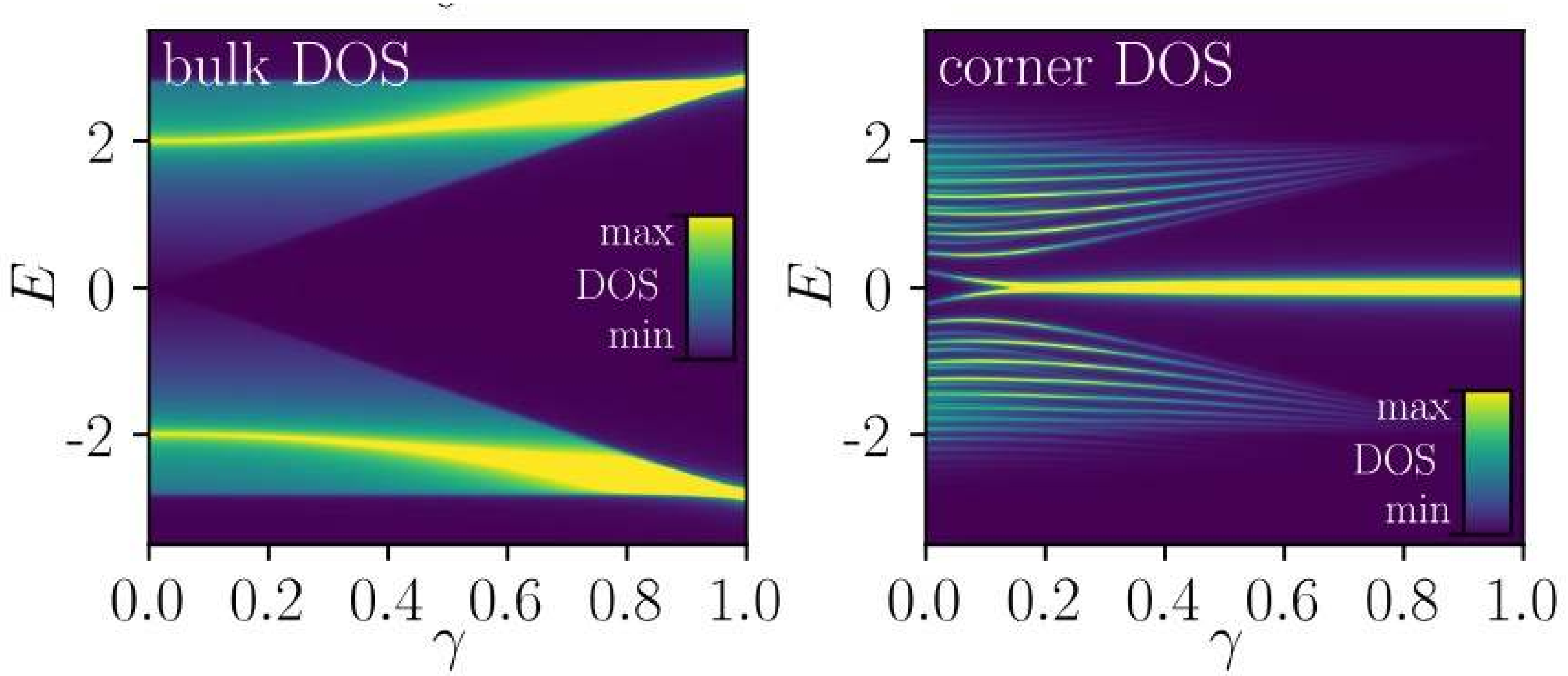
Spinon pi-flux model

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

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

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

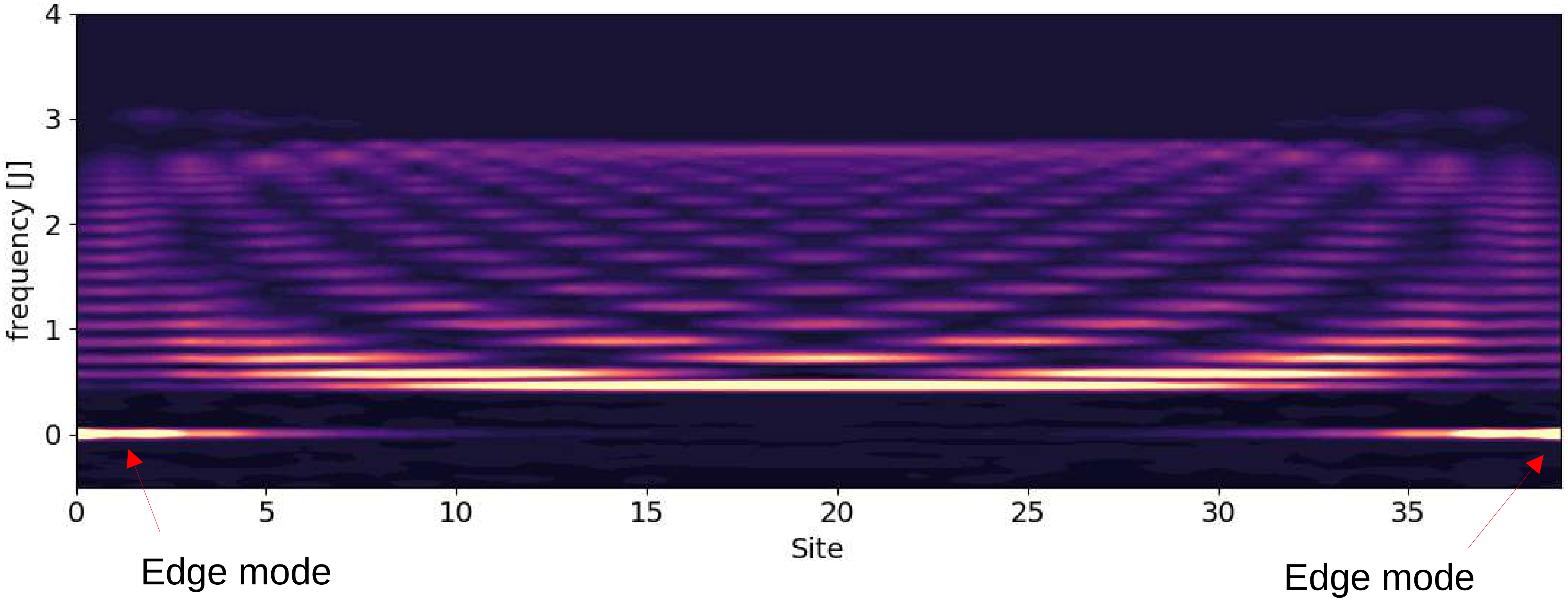
Python library for tensor-network kernel polynomial algorithms for spins, fermions, parafermions, with static solvers for Hermitian and non-Hermitian modes

```
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]))
```

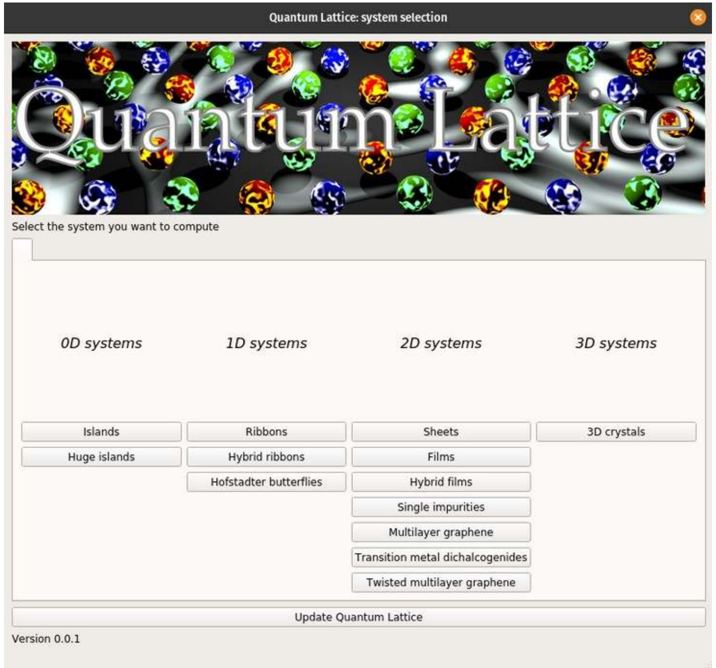
dmrgpy https://github.com/joselado/dmrgpy

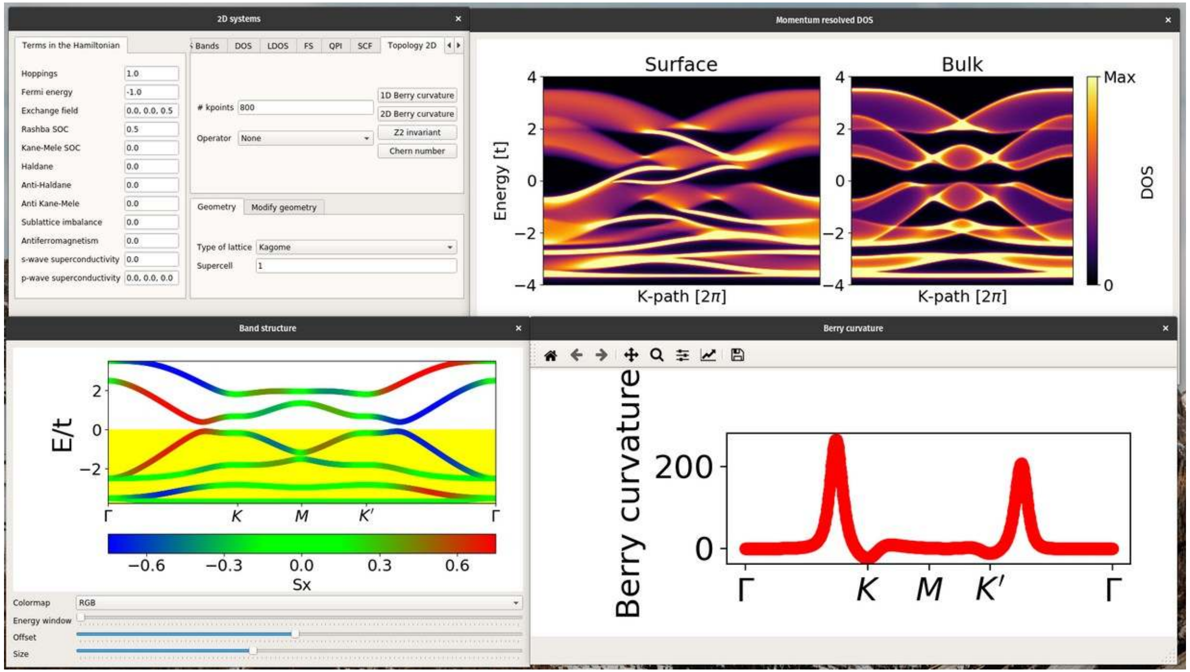
Open-source software for many-body quantum magnets

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



Quantum Lattice: A user interface to compute electronic properties



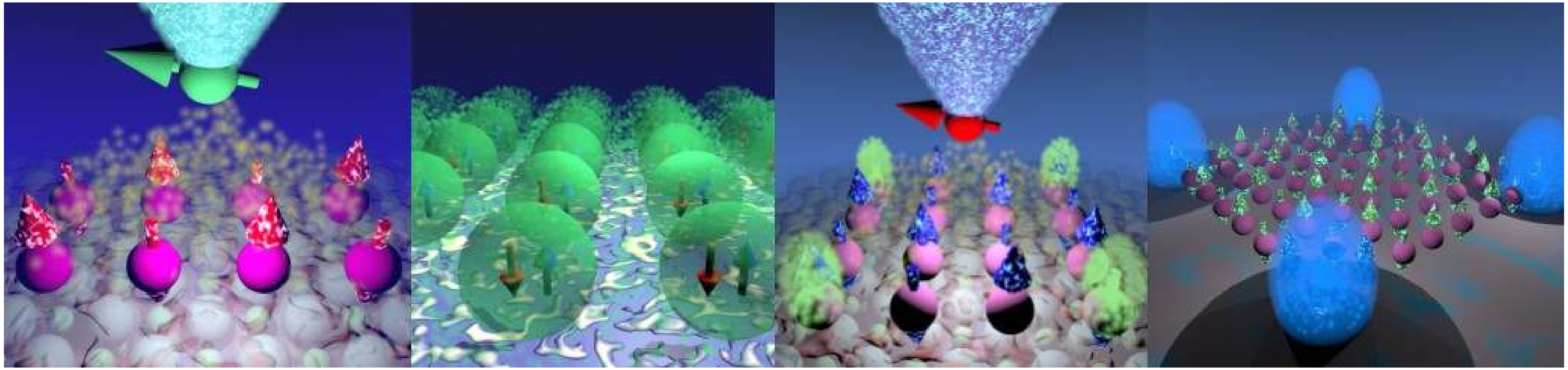


Quantum Lattice: open source interactive interface for tight binding modeling

https://github.com/joselado/quantum-lattice

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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ACADEMY OF FINLAND

J&AE JANE AND AATOS ERKKO FOUNDATION

FQF FINNISH QUANTUM FLAGSHIP

Thank you