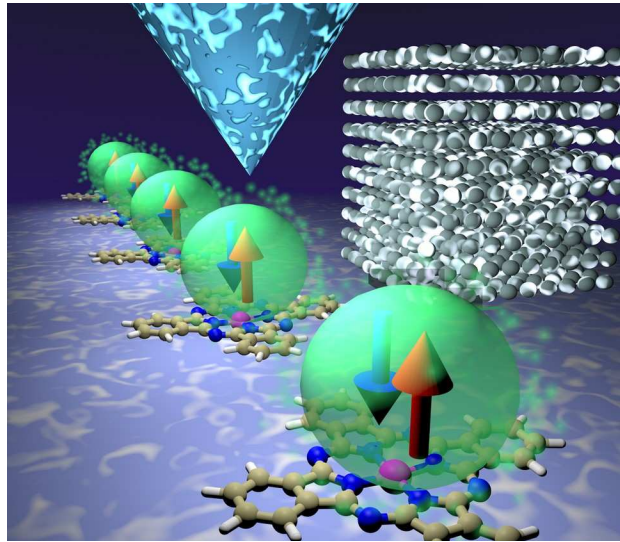


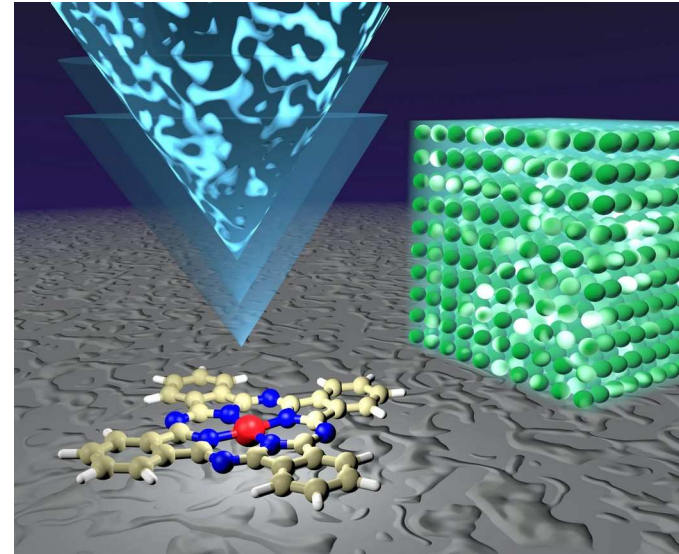
Machine learning Hamiltonians from experimental measurements

Jose Lado

Department of Applied Physics, Aalto University, Finland



Nano Letters 25, 36, 13435-13440 (2025)

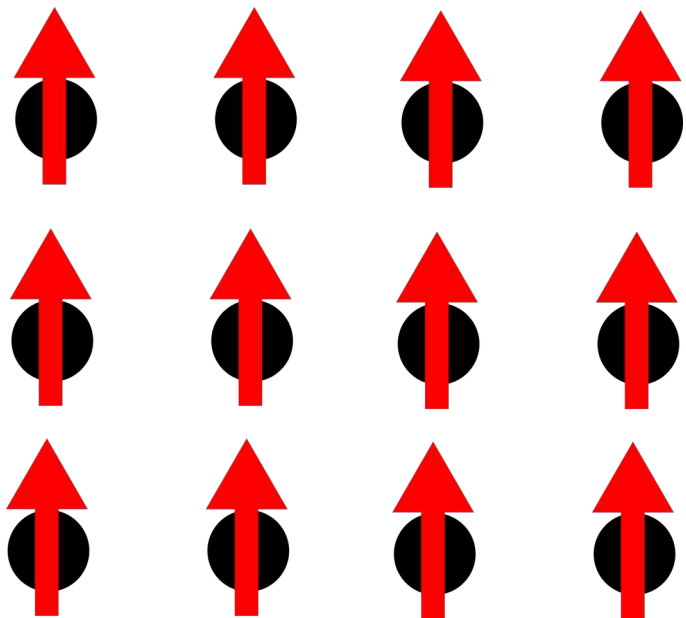


arXiv:2601.19371 (2026)

Indian Institute of Science & Aalto University Joint Webinar Series on
Quantum Technology, October 9th 2026

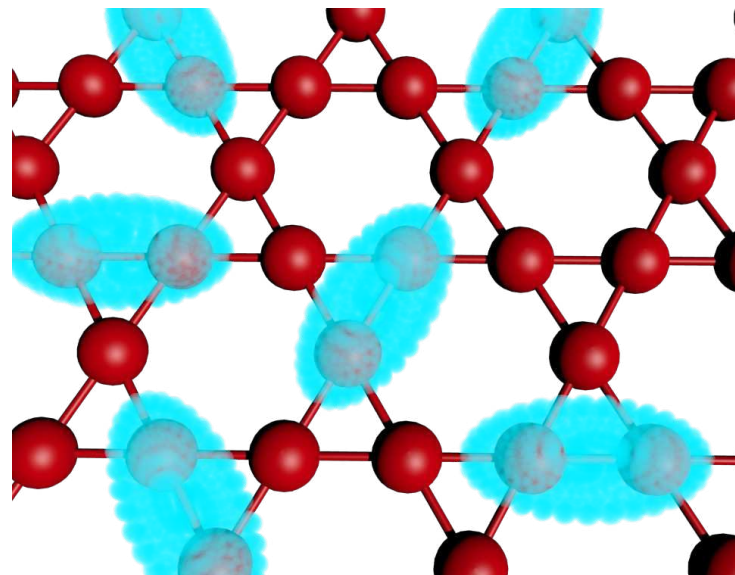
Classical and quantum magnetism

Ferromagnet & antiferromagnets



Classical ground state $\langle \vec{S}_n \rangle \neq 0$

Quantum spin-liquids



Quantum ground state $\langle \vec{S}_n \rangle = 0$

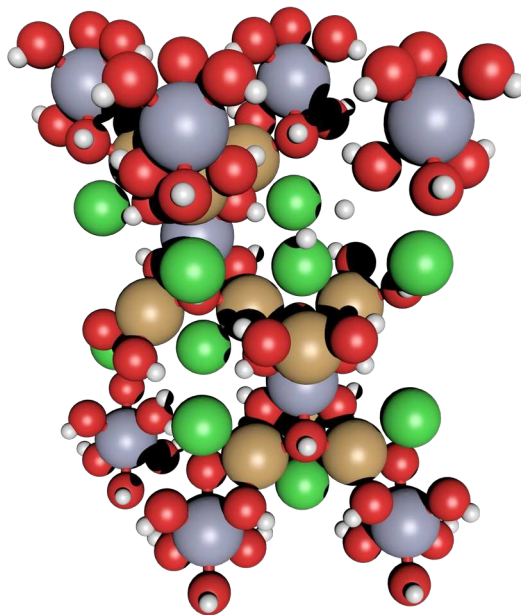
Classical and quantum magnetic materials

Ferromagnets & antiferromagnets



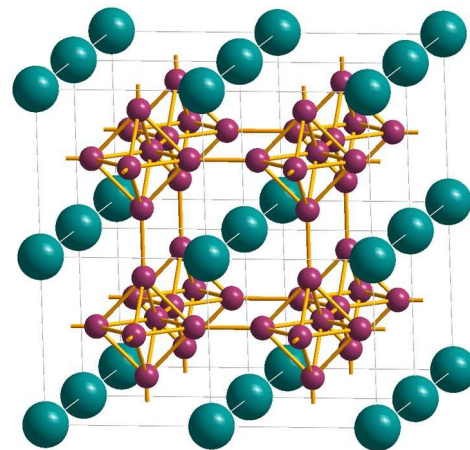
NiO_2

Quantum spin-liquids



Herbertsmithite

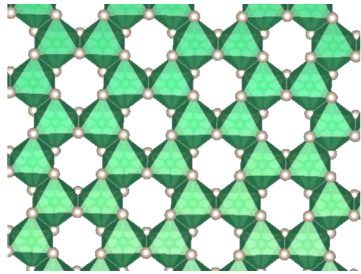
**Heavy-fermion
Kondo insulators**



SmB_6

Classical and quantum magnetic 2D materials

Ferromagnet, antiferromagnets

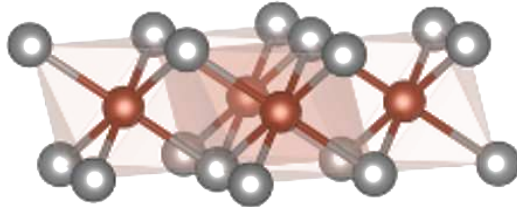


CrI_3 , CrCl_3 , CrBr_3

Nature 546, 270–273 (2017)

Break time-reversal

Multiferroics

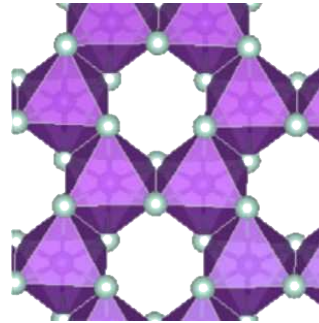


NiI_2

Nature 602, 601–605 (2022)

Break time-reversal
and inversion symmetry

Quantum spin-liquids

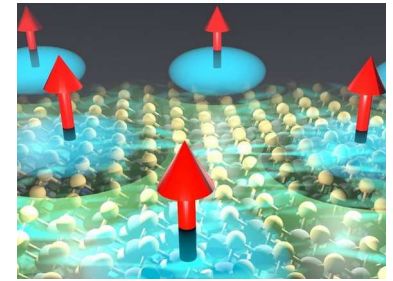


RuCl_3 , 1T-TaS_2

Nature Physics 17, 1154–1161 (2021)

Do not break time-reversal

Heavy-fermion Kondo insulators

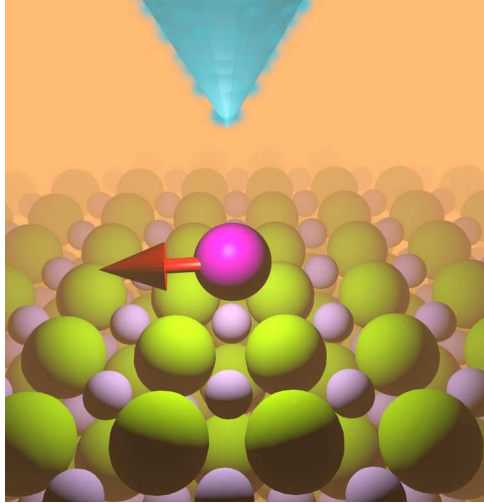


$1\text{T-TaS}_2/1\text{H-TaS}_2$

Nature 599, 582–586 (2021)

Engineering artificial quantum materials

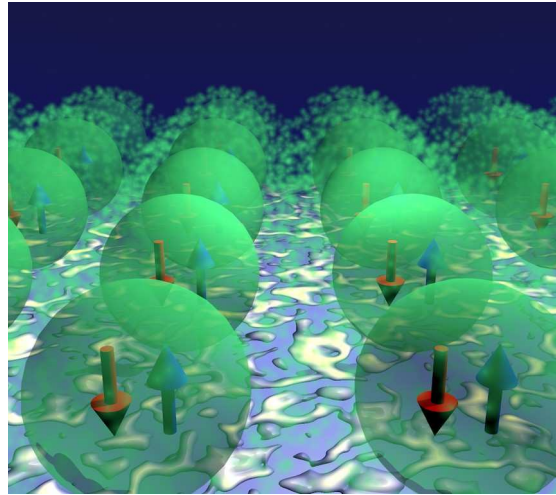
Atomic lattices



$a = 0.5 \text{ nm}$

Nature Physics 7 (9), 713-718 (2011)
Nature Physics 13 (7) 668 (2017)
Nature Nano 17 (4), 384-389 (2022)
Science 335 (6065), 196-199 (2012)

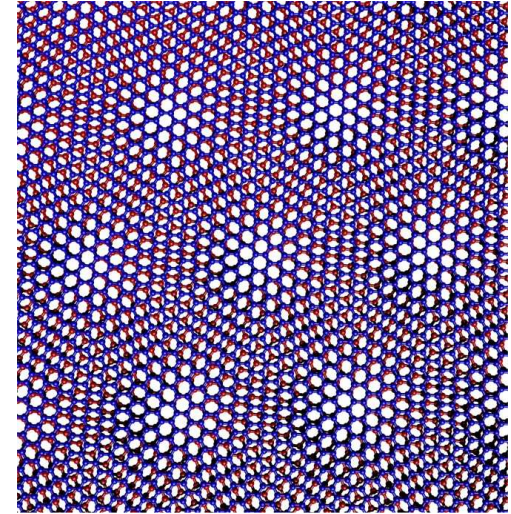
Molecular lattices



$a = 3 \text{ nm}$

Nature 408, 447-449 (2000)
Nature Rev. Mat. 5 (2), 87-104 (2020)
Nature 598, 287-292 (2021)
Phys. Rev. Lett. 130, 100401 (2023)

2D moire materials

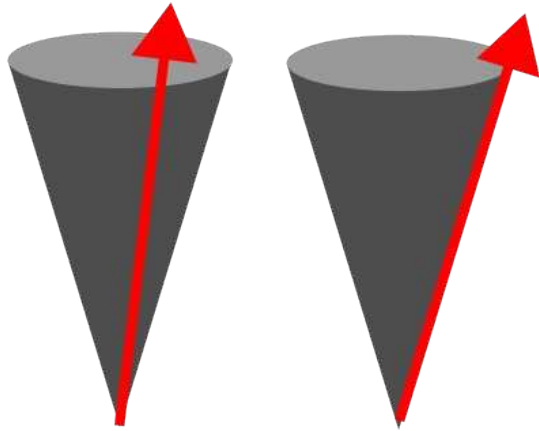


$a = 20 \text{ nm}$

Phys. Rev. Lett. 99, 256802 (2007)
Nature Physics 6, 109-113 (2010)
PNAS 108 (30) 12233-12237 (2011)
Nature 556, 80-84 (2018)

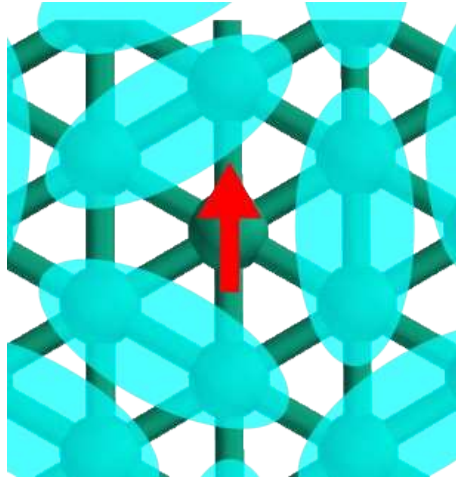
Excitations in correlated magnets

Magnons



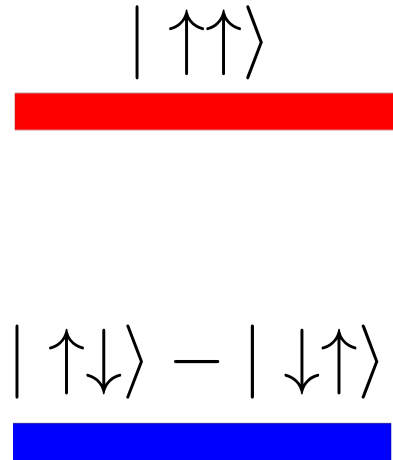
$S=1$

Spinons



$S=1/2$

Triplons



$S=1$

A minimal quantum magnet: 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

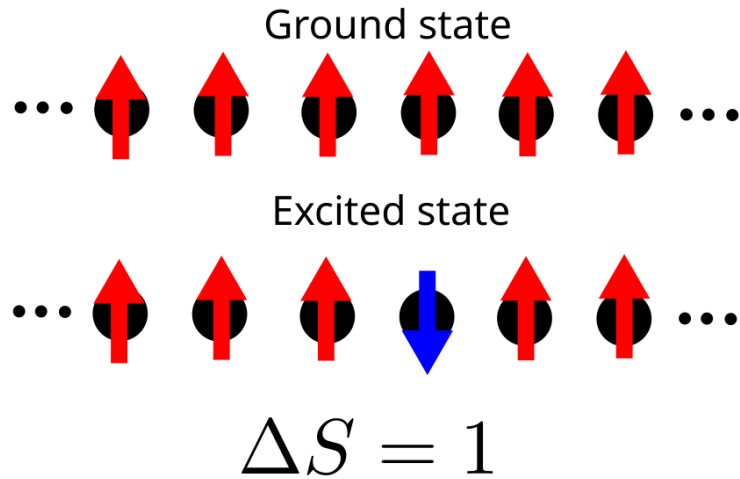
$$|GS\rangle = \frac{1}{\sqrt{2}} [|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle] \quad \langle \vec{S}_i \rangle = 0$$

The state is maximally entangled

Quantum magnets are macroscopic versions of these entangled states

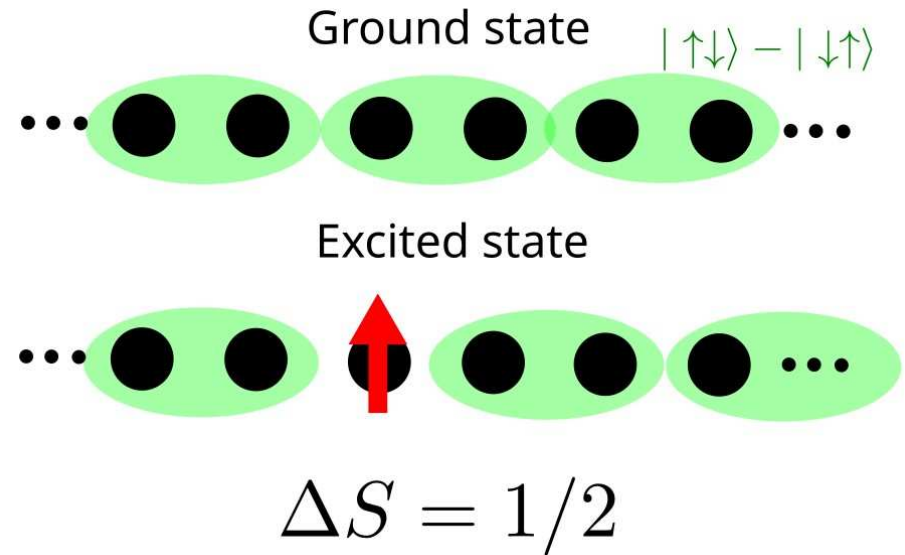
Two excitations in magnetic materials

Excitations in a symmetry broken magnet



Magnons

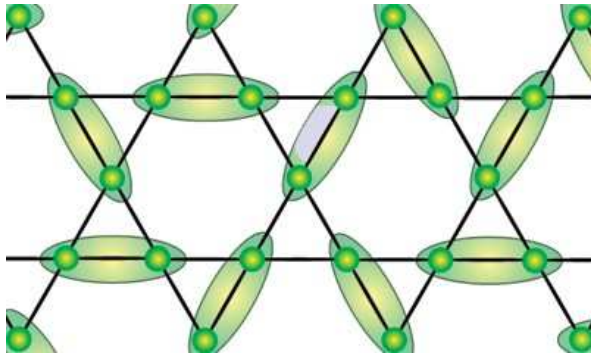
Excitations in a quantum spin liquid



Spinons

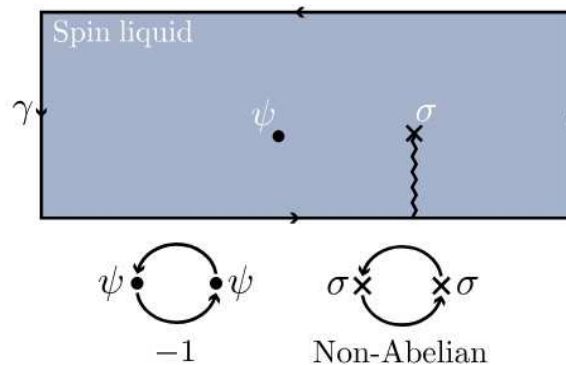
Quantum spin liquid materials: opportunity and challenge

Macroscopically entangled magnetic state



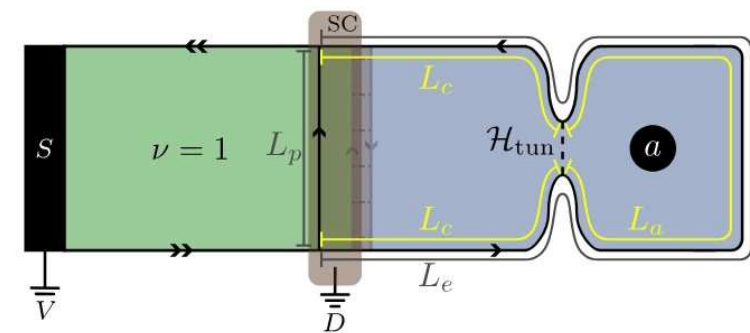
Rep. Prog. Phys. 80, 016502 (2017)

Featuring fractional excitations



Phys. Rev. X 10, 031014 (2020)

Potential candidates for topological quantum computing



Phys. Rev. X 12, 011034 (2022)

Many potential QSL candidates (Herbertsmithite, 1T-TaS₂, RuCl₃)

However, quantum spin liquids are exceptionally challenging to identify experimentally

How can we learn the microscopic description of quantum magnets?

The problem of Hamiltonian learning

If we measure a quantum magnet, how can we obtain its microscopic description?

Conventional workflow in theoretical physics

Solve the Hamiltonian

$$H \xrightarrow{\text{Many-body solver}} \langle \Psi | O | \Psi \rangle$$

Compute an observable

The problem we often find experimentally

Measure an observable

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

Determine its Hamiltonian

How can we extract a complex Hamiltonian from its physical observables?

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

Supervised
learning



"Dog"

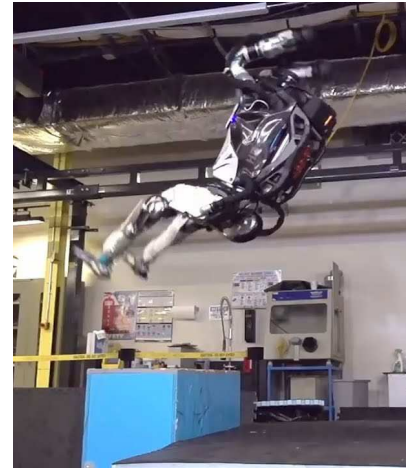
Labeled prediction

Generative
learning



Probability Modeling

Reinforcement
learning



Reward-based decision

(and others)

Two strategies for Hamiltonian learning

Uniquely defined problems

$$dI/dV \longrightarrow \mathcal{H}$$

A set of experiments is consistent with a single Hamiltonian

Supervised learning

Nano Letters 25, 36, 13435-13440 (2025)
arXiv:2601.19371 (2026)

Multiply-defined problems

$$dI/dV \begin{cases} \longrightarrow \mathcal{H}_1 \\ \longrightarrow \mathcal{H}_2 \\ \longrightarrow \mathcal{H}_3 \end{cases}$$

A set of experiments constrain the Hamiltonian, but it is non-unique

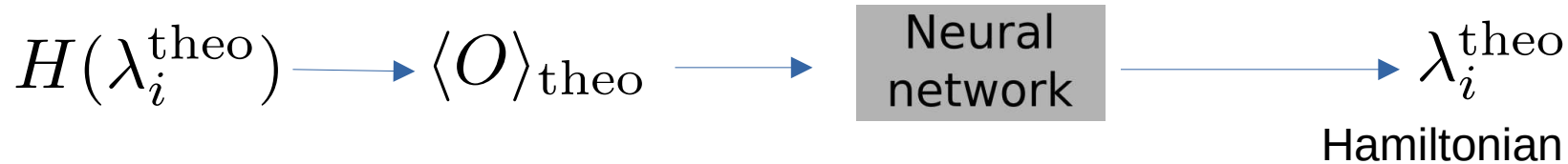
Generative learning

Phys. Rev. Applied 20, 044081 (2023)
to appear (2026)

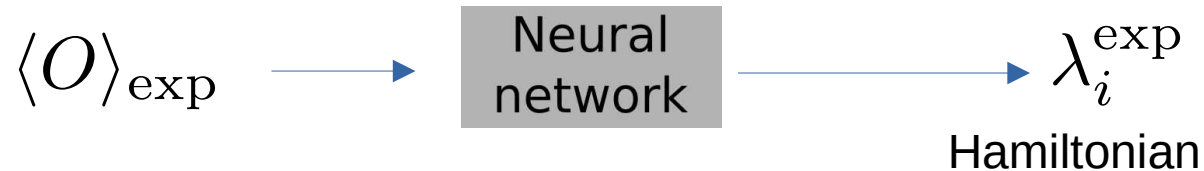
Supervised Hamiltonian learning: combining theory and experiment

Train a machine learning algorithm with simulated quantum many-body theory data

so that the parameters of each Hamiltonian are explicitly know



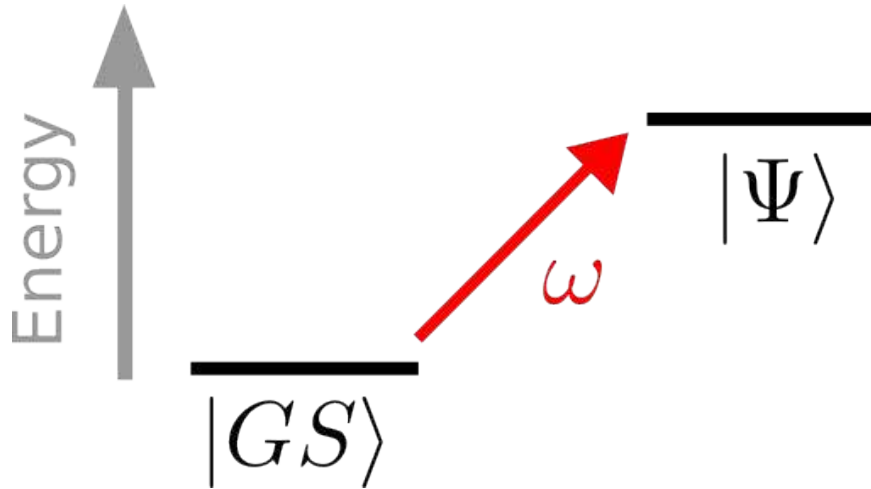
With the trained algorithm, evaluated in experimental data to extract the parameters



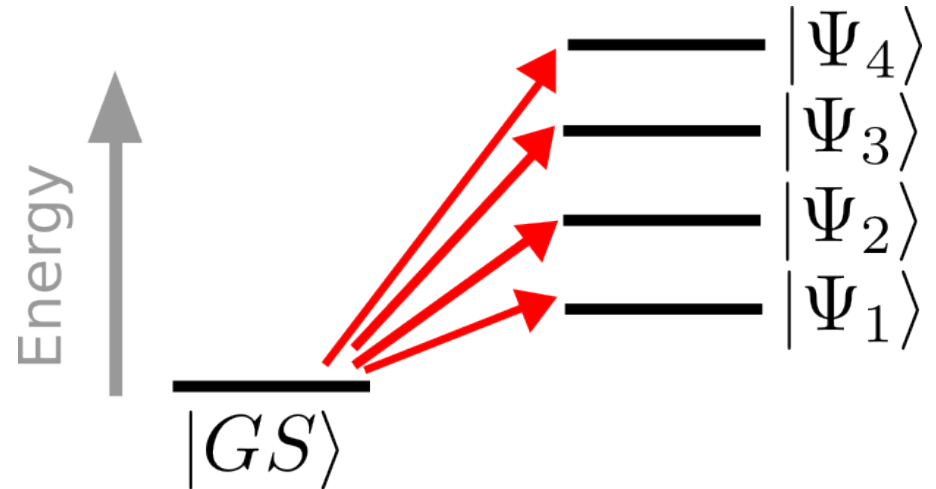
**This strategy combines quantum many-body solvers,
machine learning, and experimental measurements**

Spin excitations in collective quantum magnets

Minimal quantum spin system



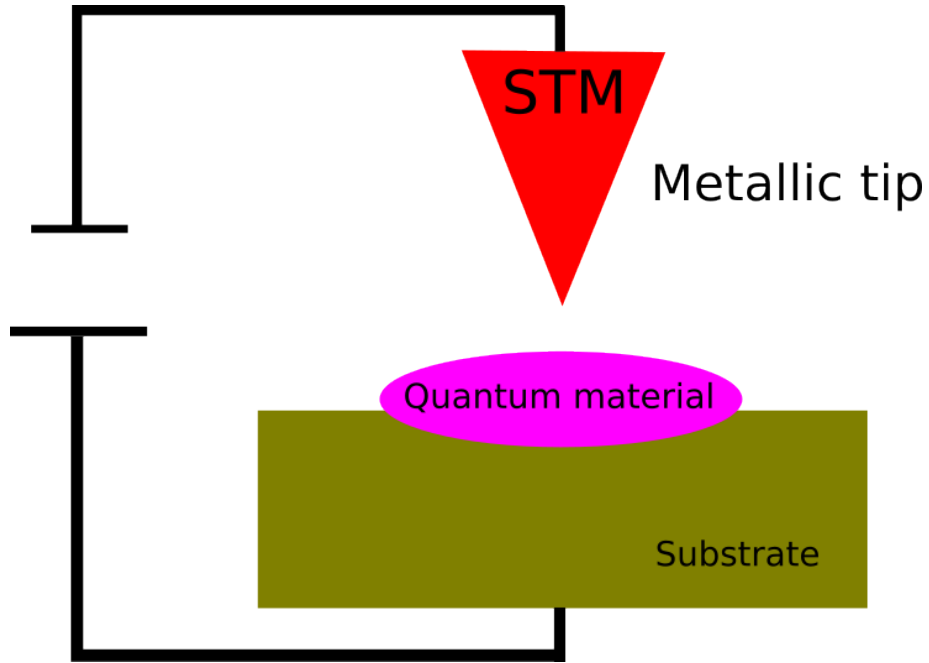
Complex quantum many-body system



Spin excitations in quantum materials are described by the dynamical spin correlator

That can be measured with scanning tunneling microscopy

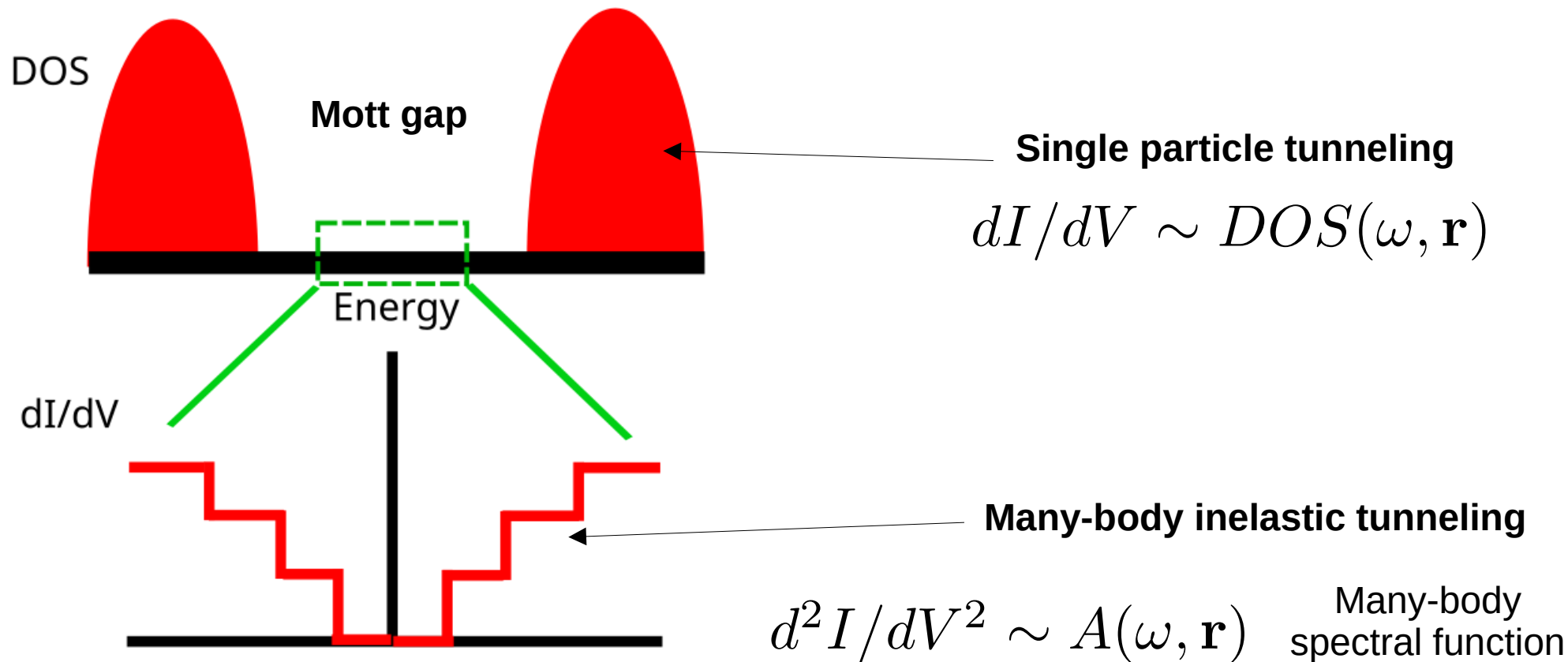
Spectroscopy atomic-scale quantum matter with STM



Atomic real-space resolution
Energy/frequency and time resolution

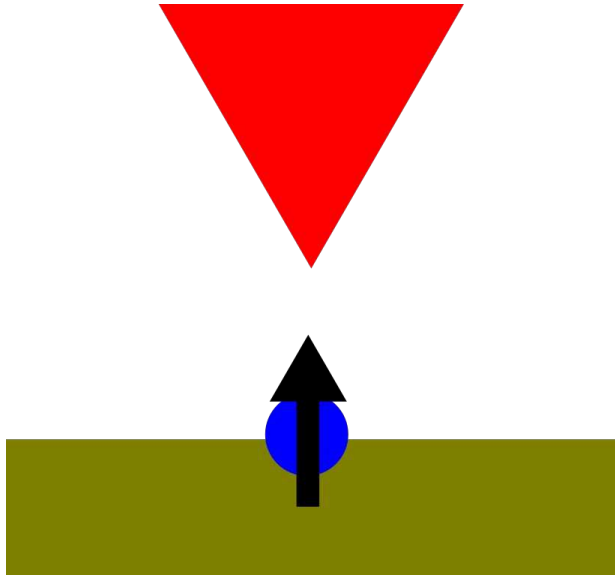
- Electronic states
- Phonons
- Superconducting pairing
- Orbital order
- Spin excitations

Single particle VS many-body excitations in STM



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

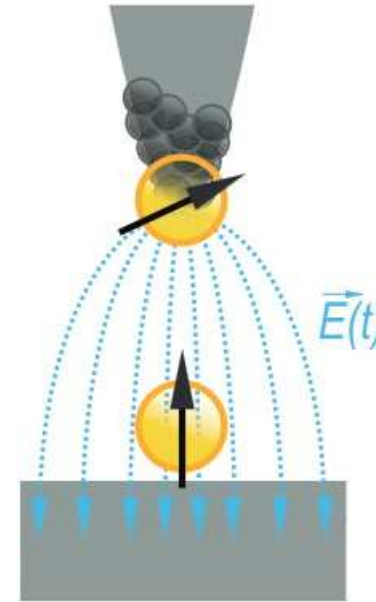
Inelastic electron tunneling spectroscopy (IETS)



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

Without spin-polarized tip

Electrically driven electron spin resonance (ESR)



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

With spin-polarized tip

Generating the training data: Solving the quantum many-body problem

Let us take a simple many-body problem

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

A typical wavefunction is written as

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

We need to determine in total 2^L coefficients

Is there an efficient way of storing so many coefficients?

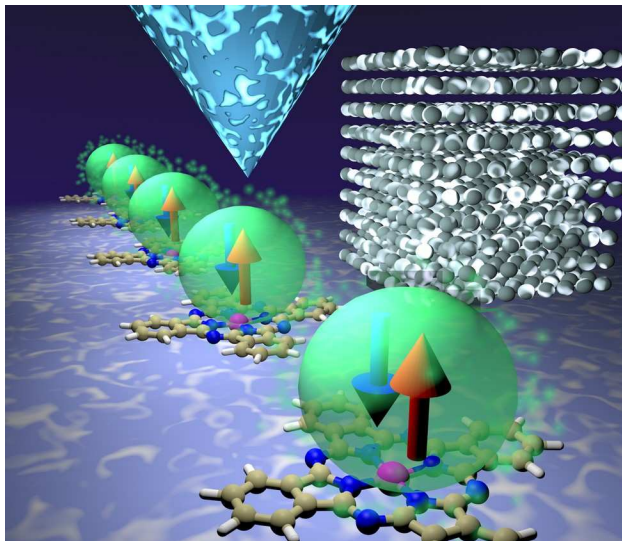
And ultimately compute the dynamical spin correlator

Dealing with very large spaces with tensor networks

A many-body wavefunction is a very high dimensional object (2^L coefficients)

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

Tensor-networks allow “compressing” exponentially large information with linear resources



“True wavefunction”



“Tensor-network wavefunction”

Dealing with very large spaces with tensor networks

Typical many-body wavefunction

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

Tensor networks allow parametrizing many-body wavefunctions as

$$|\Psi\rangle = \sum_{\{s\}} M_1^{(s_1)} M_2^{(s_2)} \dots M_N^{(s_N)} |s_1 s_2 \dots s_N\rangle$$

$L\chi^2$ parameters

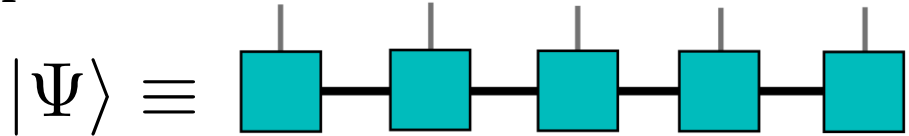


Tensor networks allow to drastically reduce the memory required to store a many-body state

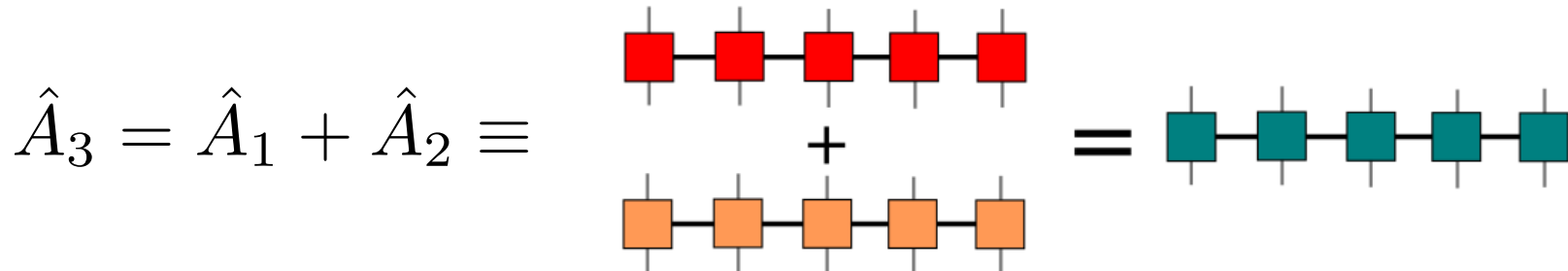
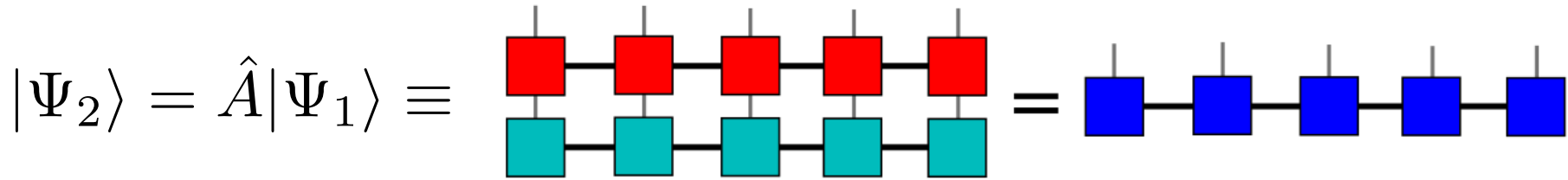
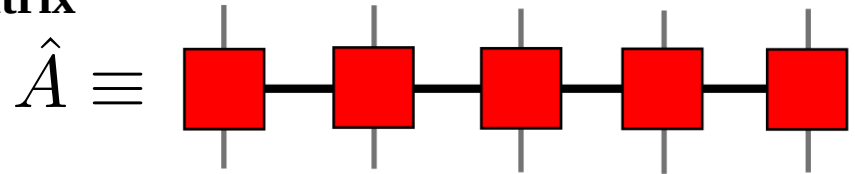
Exponentially large algebra with tensor networks

Tensor network allow to (approximately) operate in exponentially large vector spaces

vector



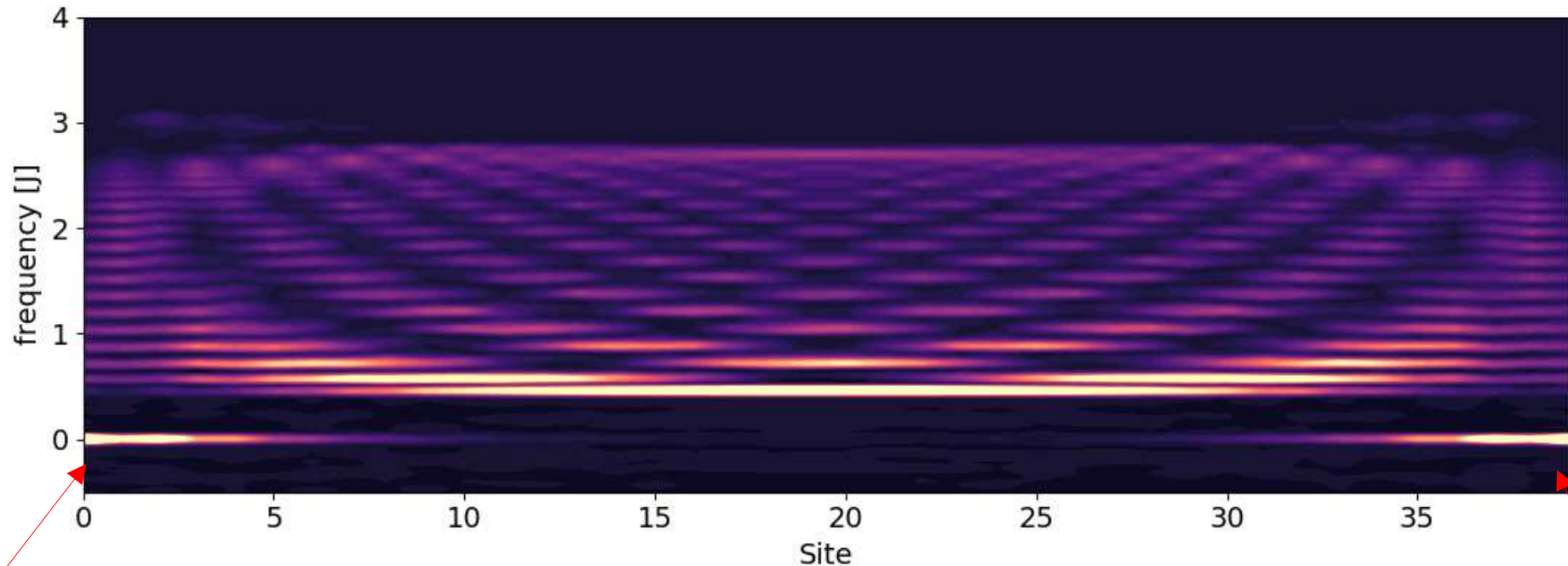
matrix



This allows us to compute observables in generic quantum many-body problems

Dynamical spectral functions in a 1D topological quantum magnet

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



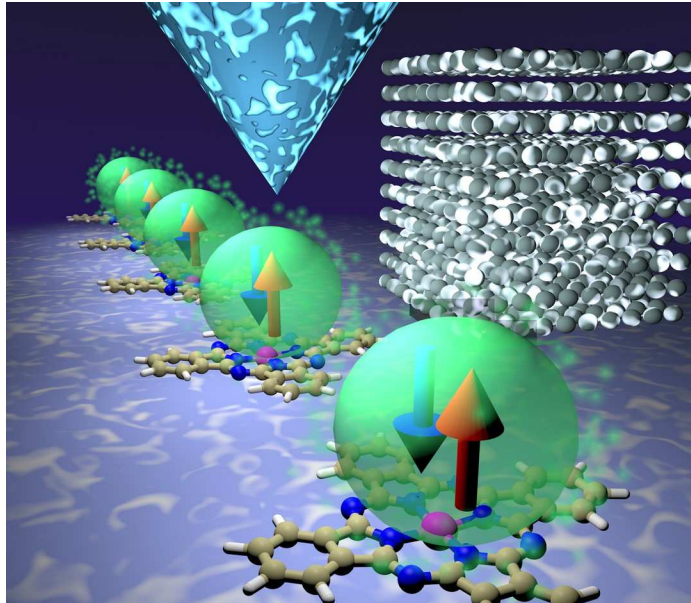
Edge mode

Open source software for spin models with tensor networks
<https://github.com/joselado/dmrgpy>

Edge mode

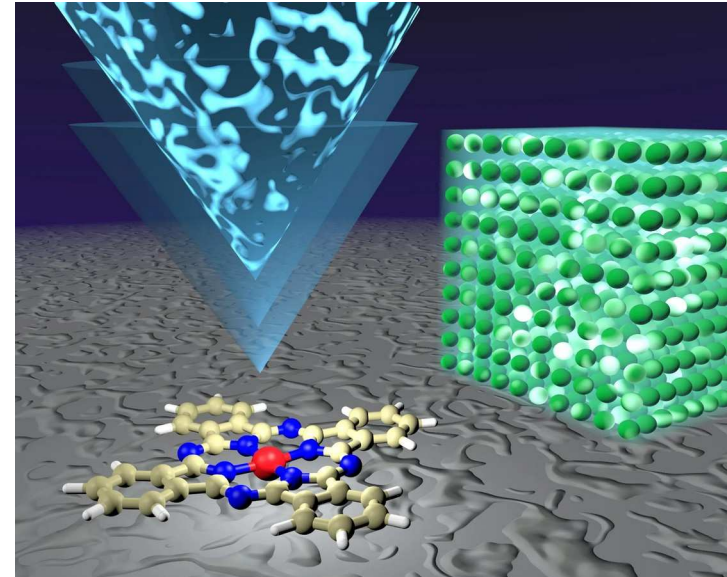
Hamiltonian learning correlated system from inelastic STM spectroscopy

**Hamiltonian learning from
spin excitation**



Phys. Rev. Lett. 131, 086701 (2023)
Nano Letters 25, 36, 13435-13440 (2025)

**Hamiltonian learning from
setpoint dependent spectroscopy**



arXiv:2601.19371 (2026)

Hamiltonian learning correlated system from inelastic STM spectroscopy

Rouven Koch



Greta Lupi



Mohammad Amini



Robert Drost



Shawulienu
Kezilebieke



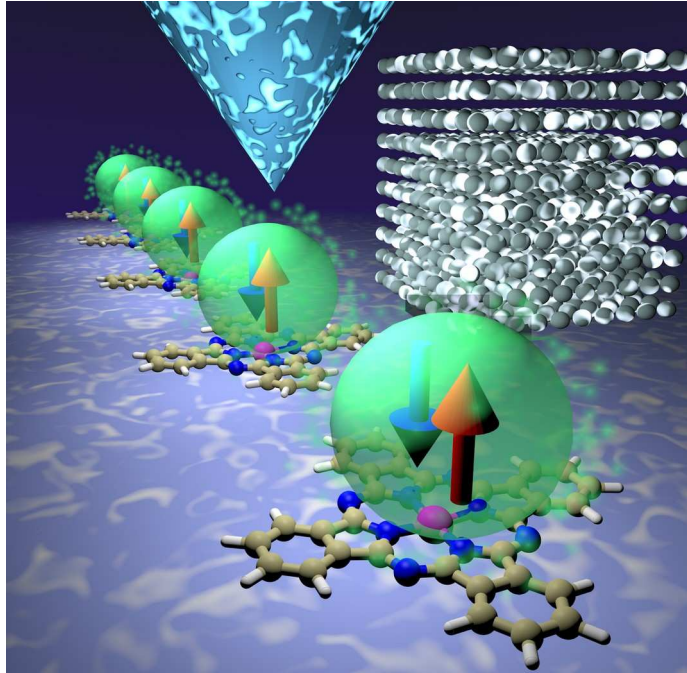
Adolfo Fumega



Peter Liljeroth



Hamiltonian learning triplons in a molecular quantum magnet



Rouven Koch



Robert Drost



Peter Liljeroth

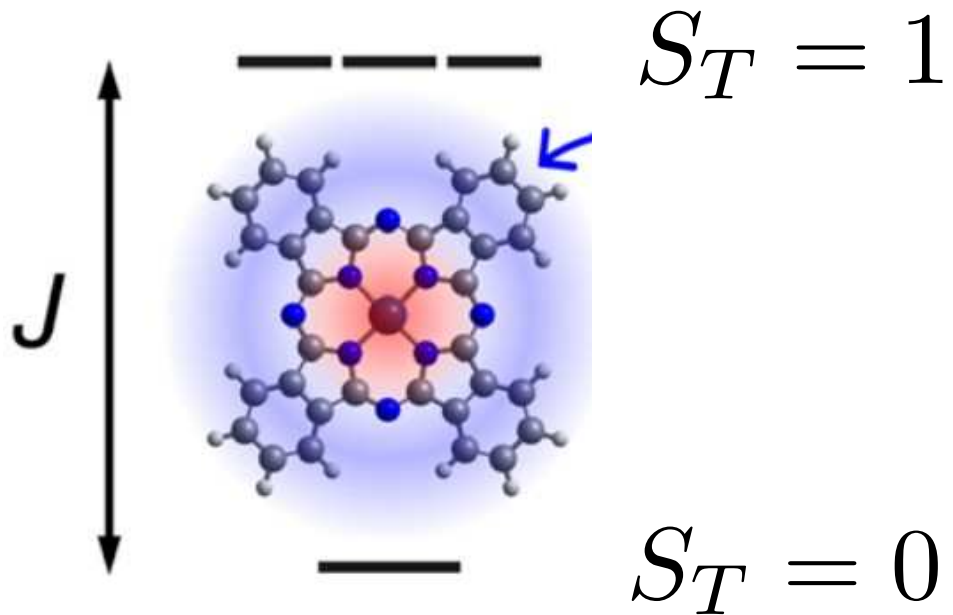


Shawulienу Kezilebieke



Phys. Rev. Lett. 131, 086701 (2023)
Nano Letters 25, 36, 13435-13440 (2025)

Triplet excitations in a molecule

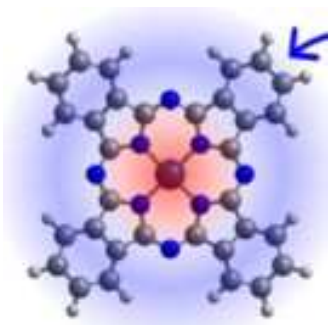


Internal antiferromagnetic coupling

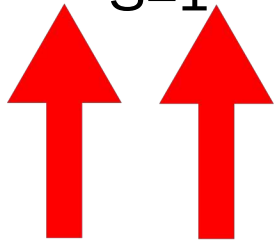
$$H = J \mathbf{S} \cdot \mathbf{K}$$

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

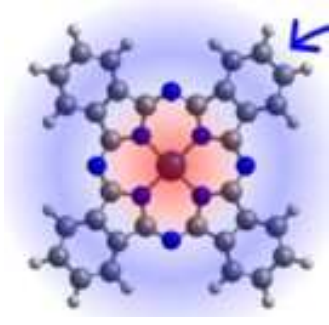
Triplons in a dimer



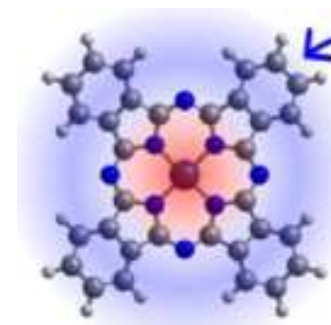
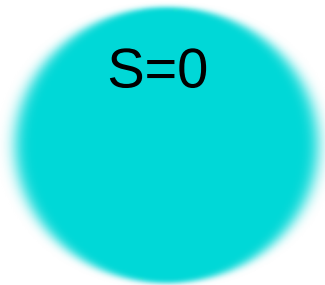
$S=1$



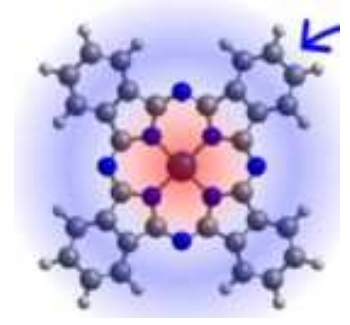
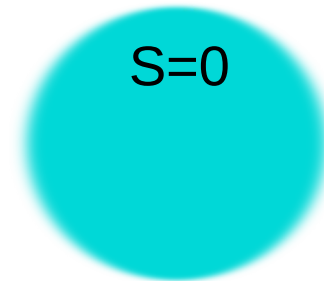
A triplet in the first molecule



$S=0$



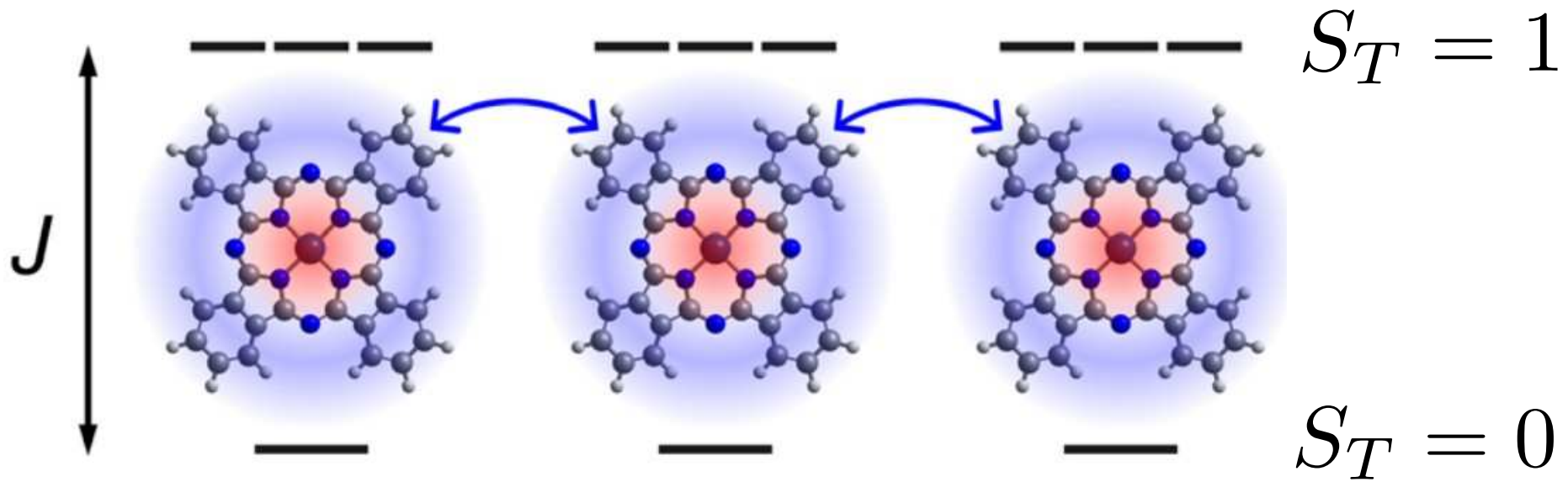
$S=1$



Can jump to the second molecule

Exchange coupling between molecules leads to propagating triplon excitations

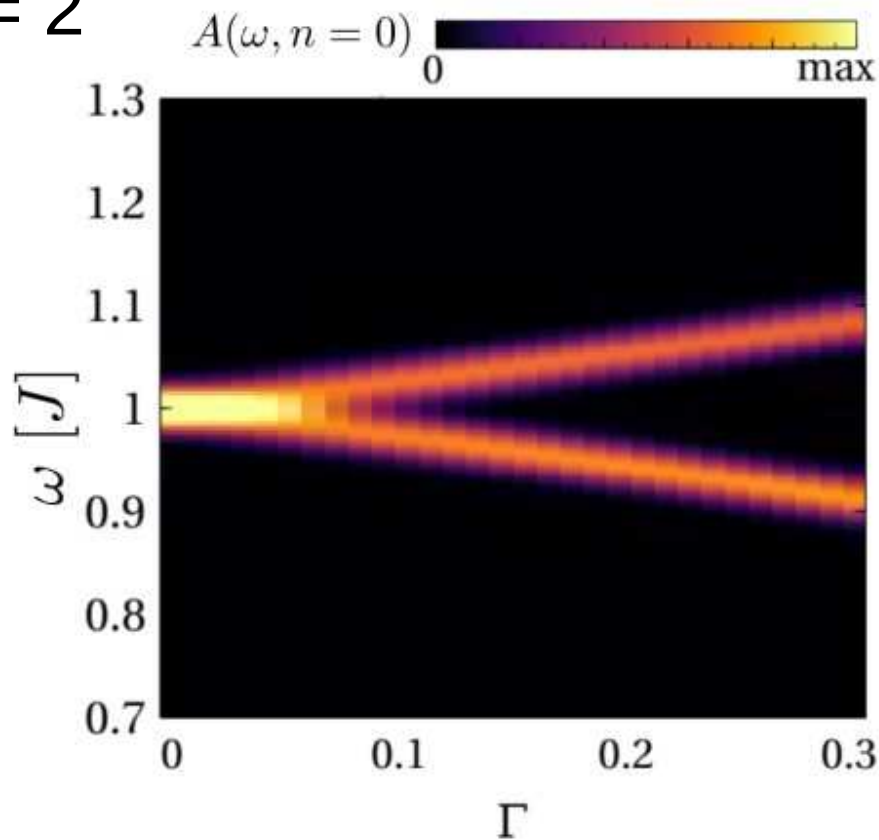
A chain of triplons



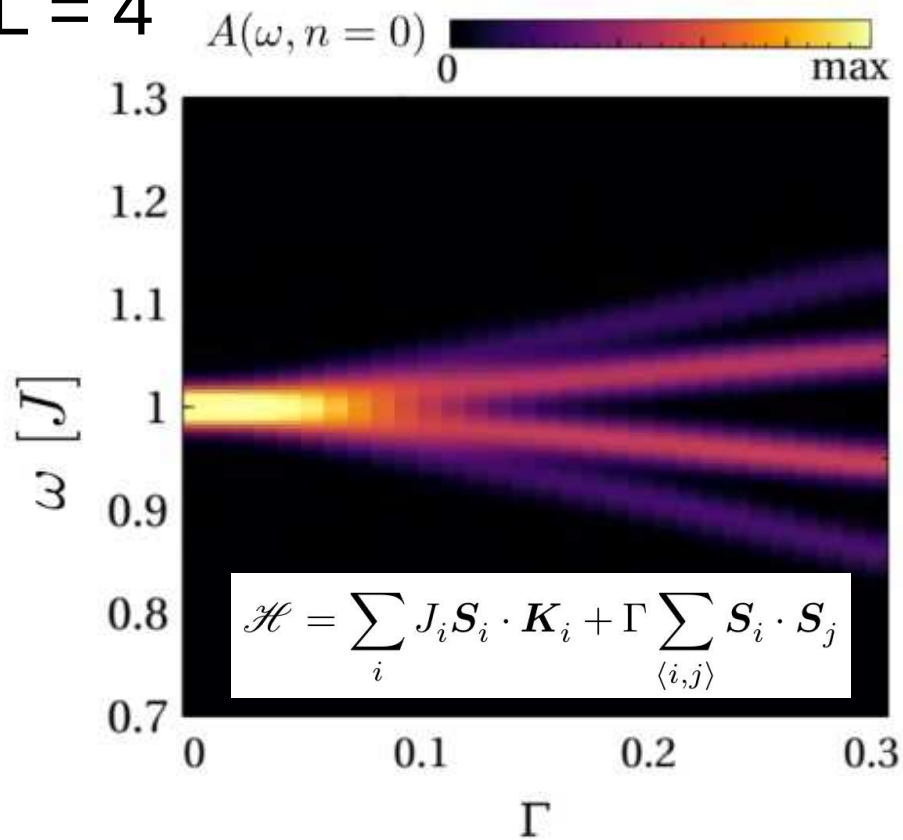
$$\mathcal{H} = \sum_i J_i \mathbf{S}_i \cdot \mathbf{K}_i + \Gamma \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

Chains of triplons

L = 2

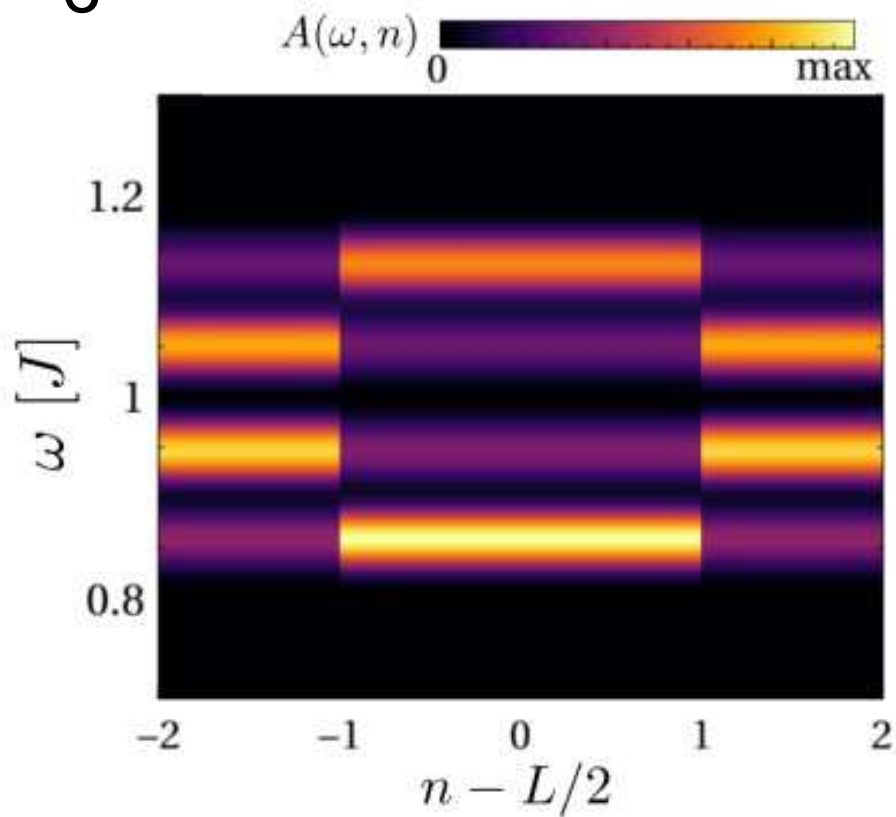


L = 4

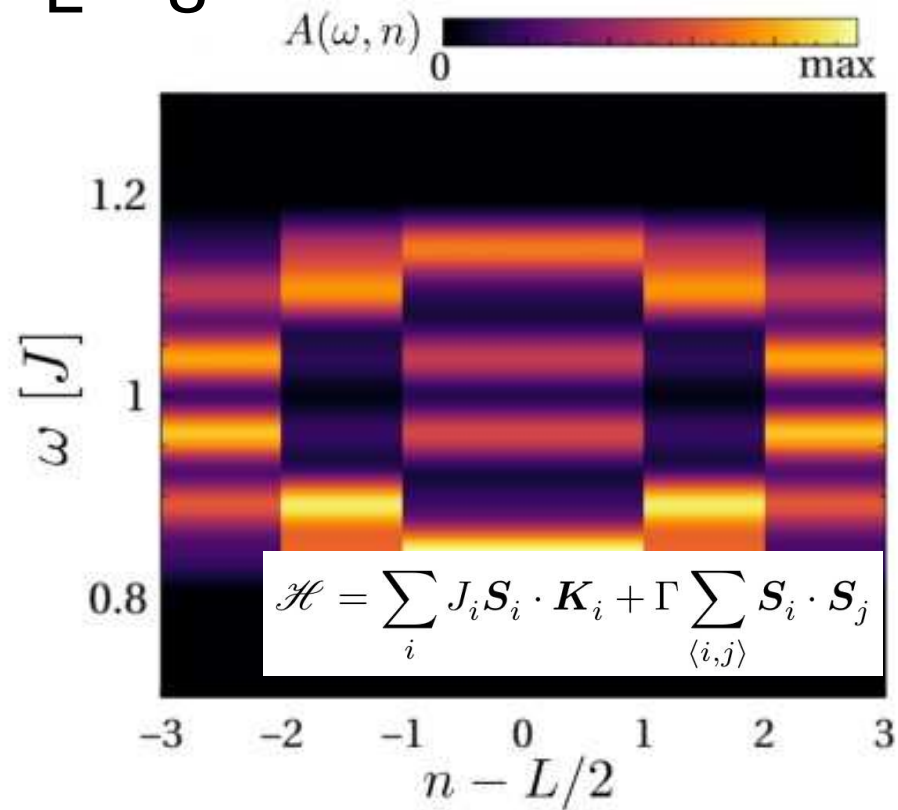


Chains of triplons

$L = 6$



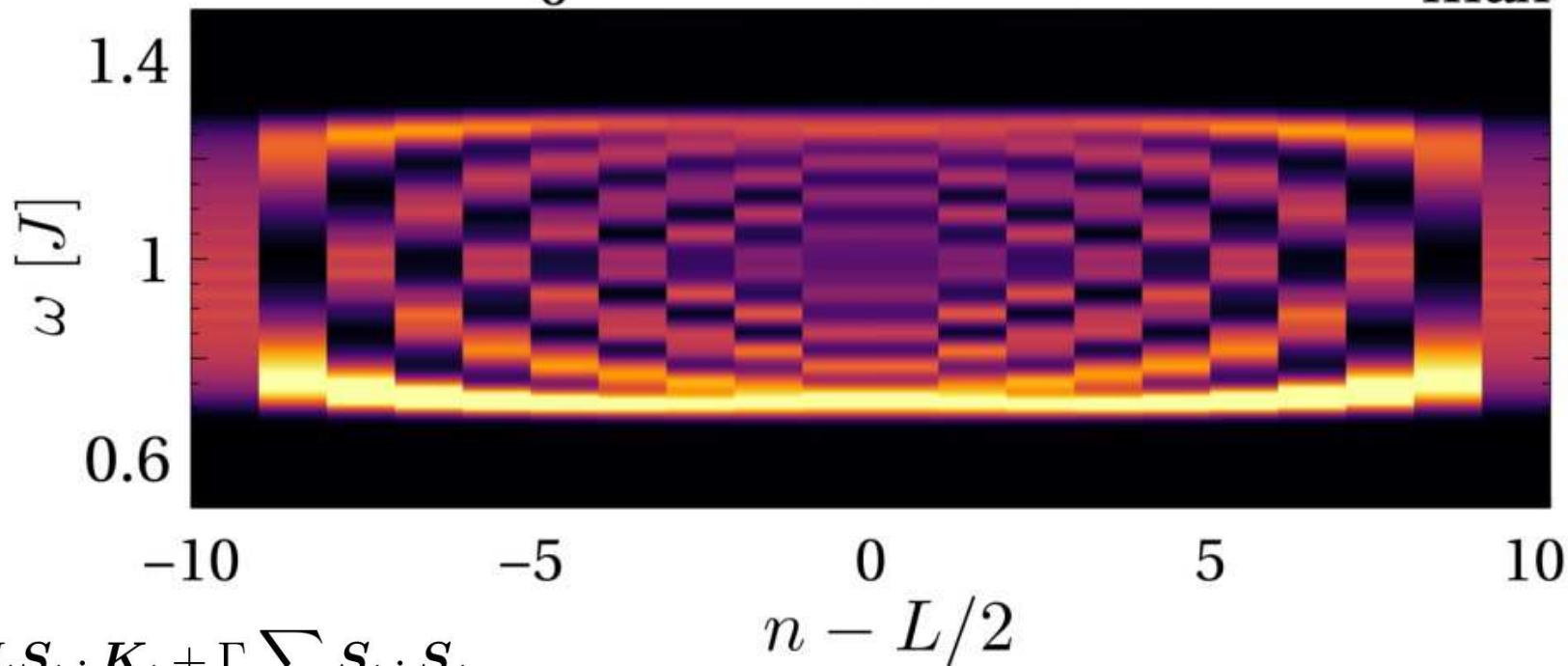
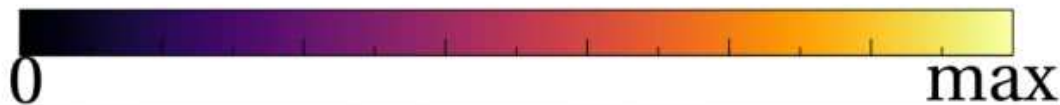
$L = 8$



Chains of triplons

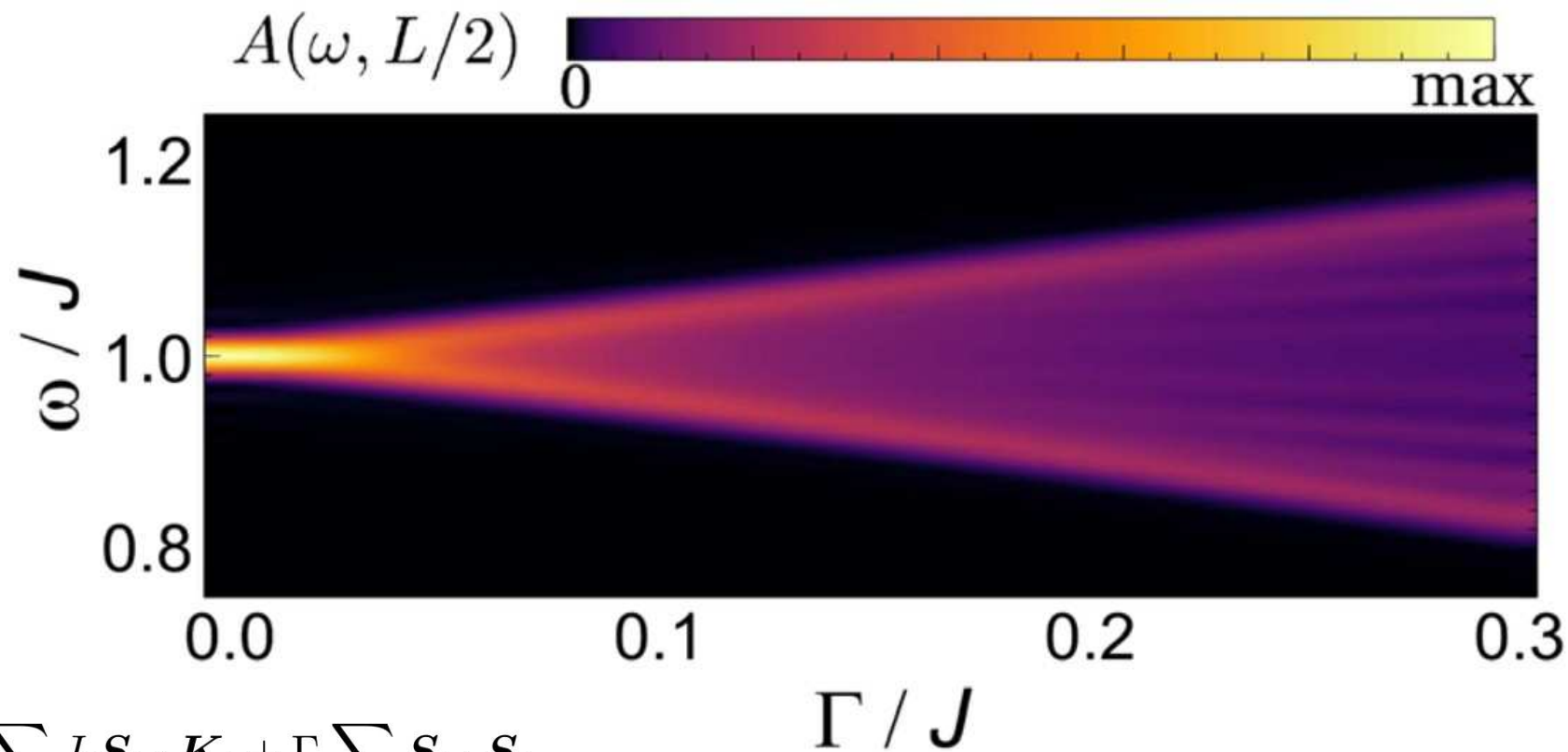
$L = 20$

$A(\omega, n)$



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

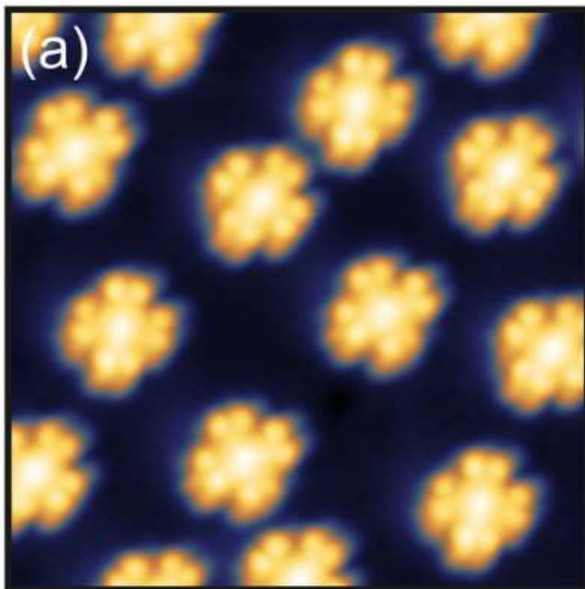
Chains of triplons



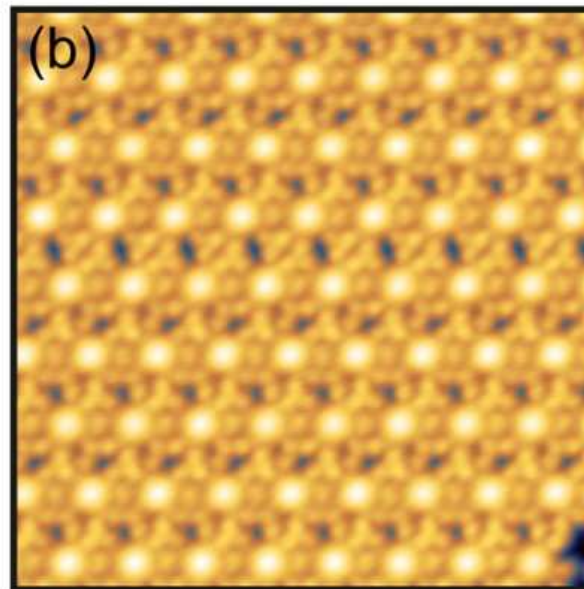
$$\mathcal{H} = \sum_i J_i \mathbf{S}_i \cdot \mathbf{K}_i + \Gamma \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

0D, 1D and 2D arrays

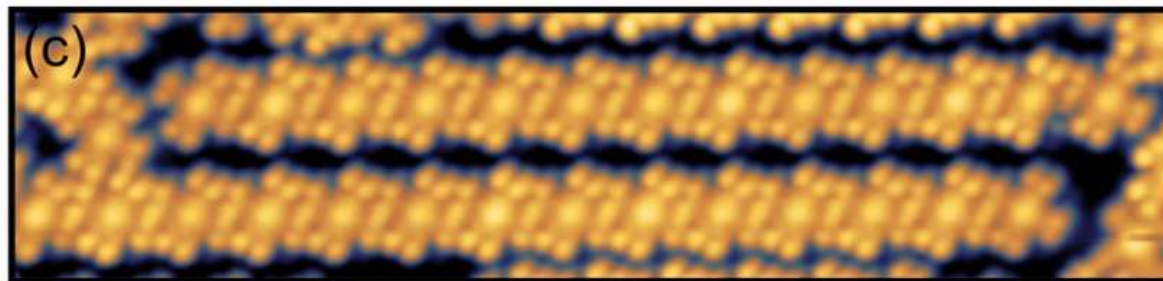
0D



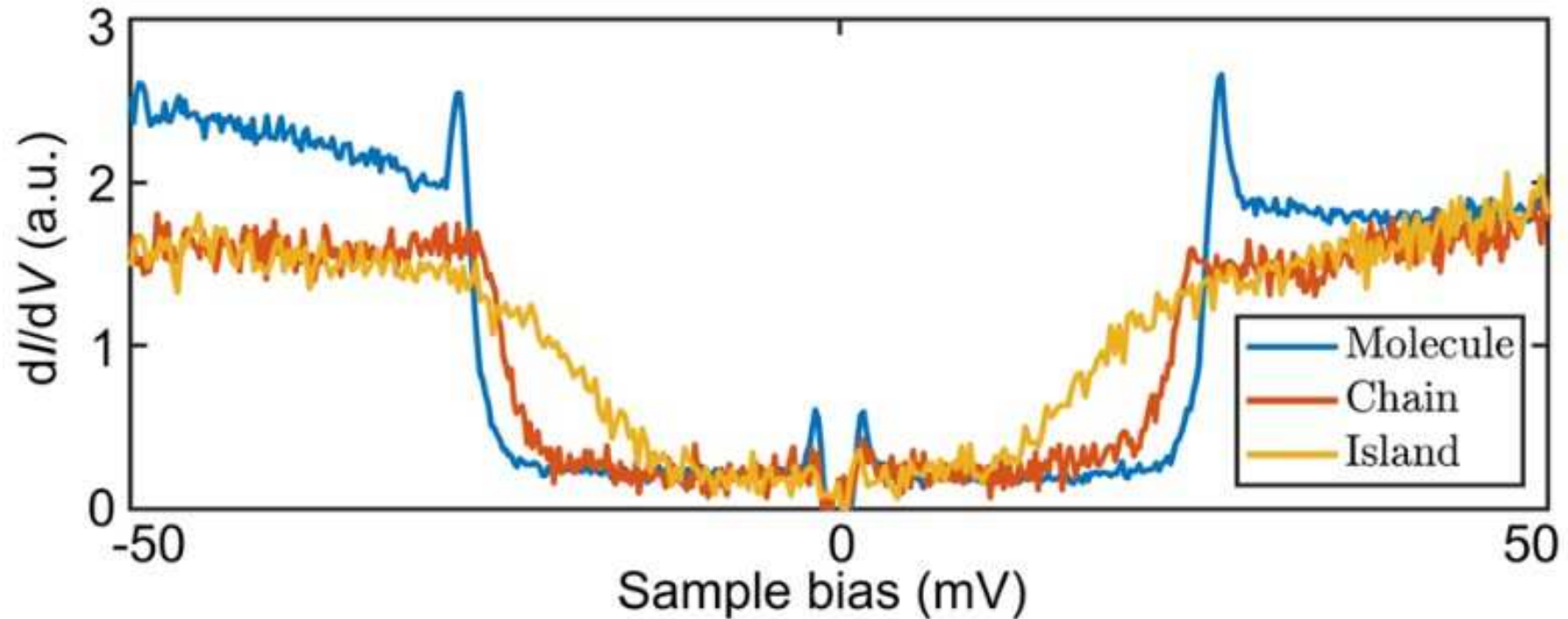
2D



1D

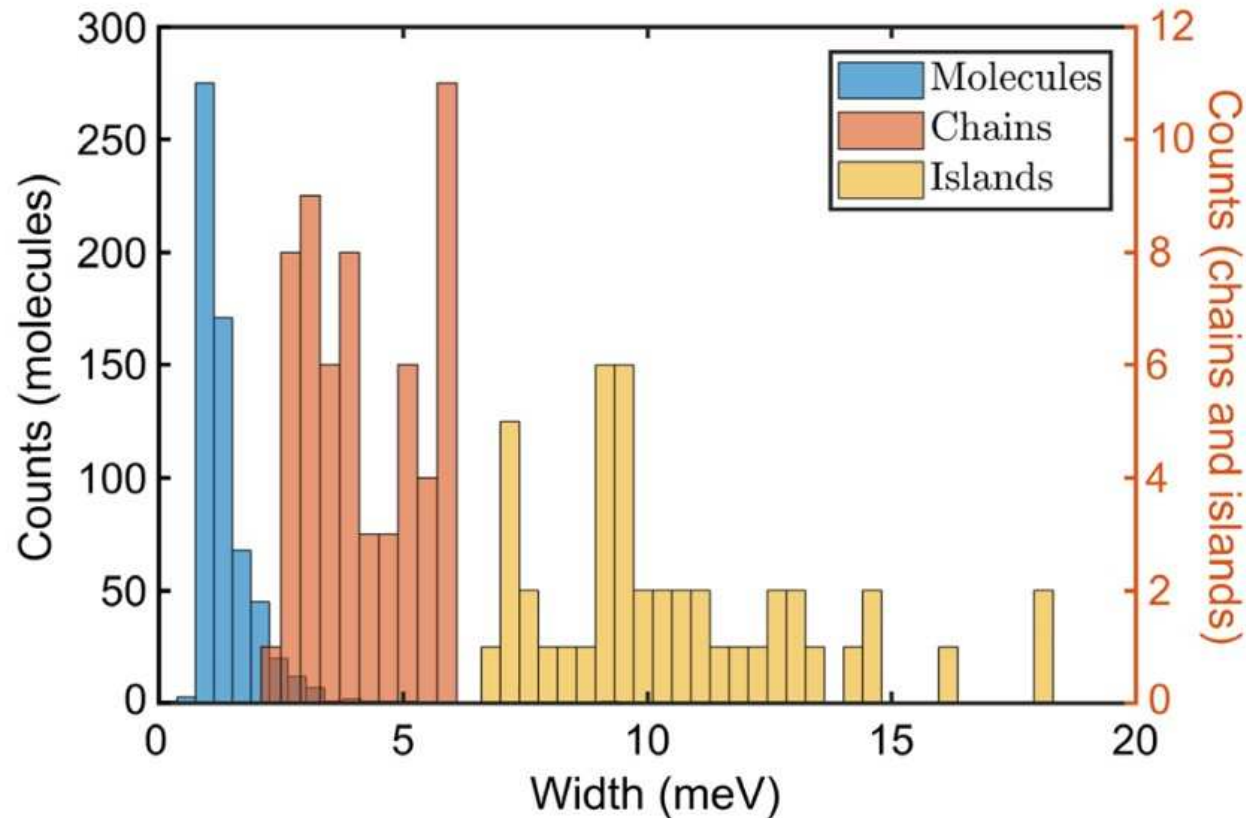


Inelastic excitations for 0D, 1D and 2D arrays



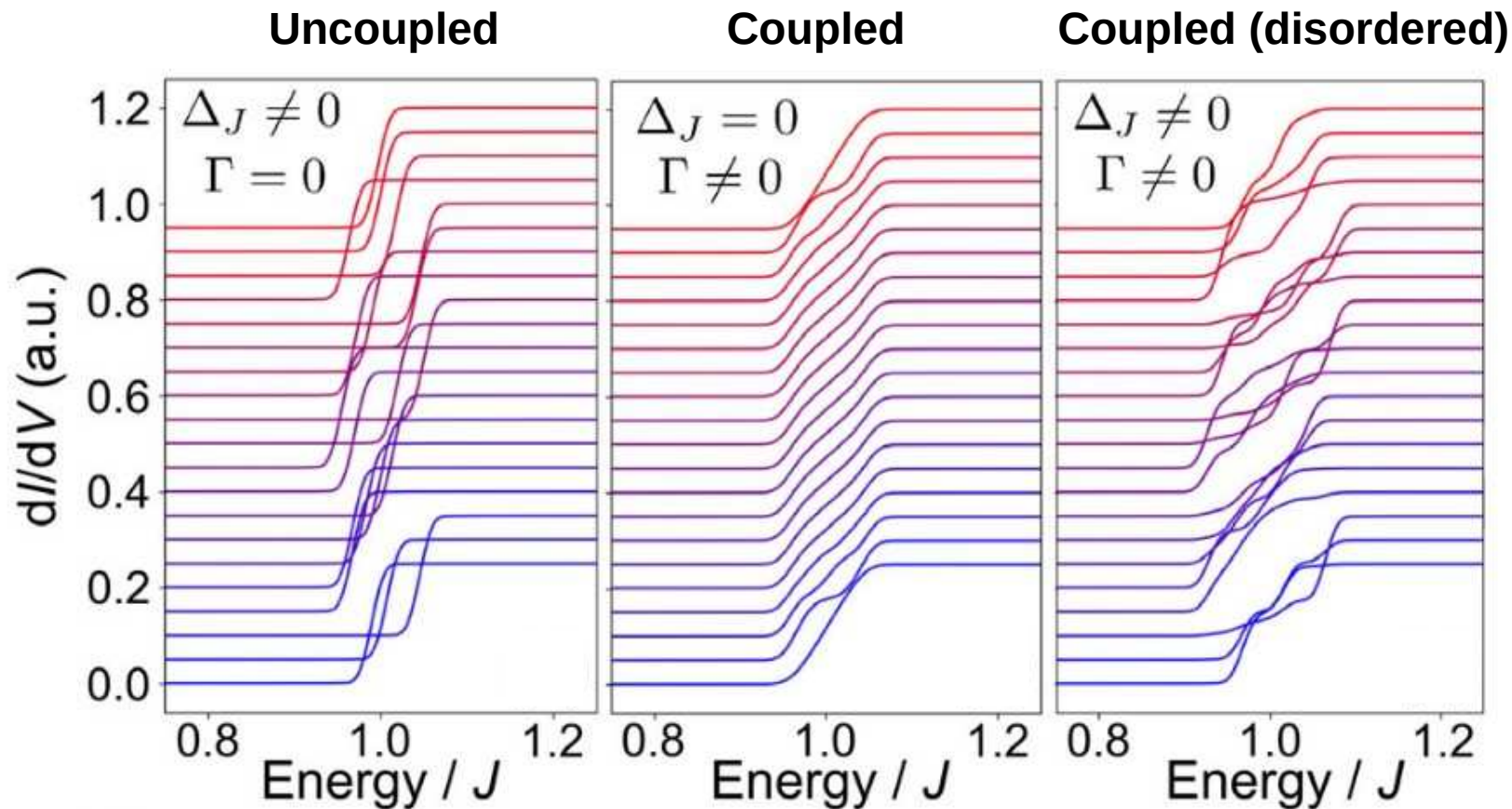
The width of the step is bigger for islands than for molecules

Statistic of the inelastic steps

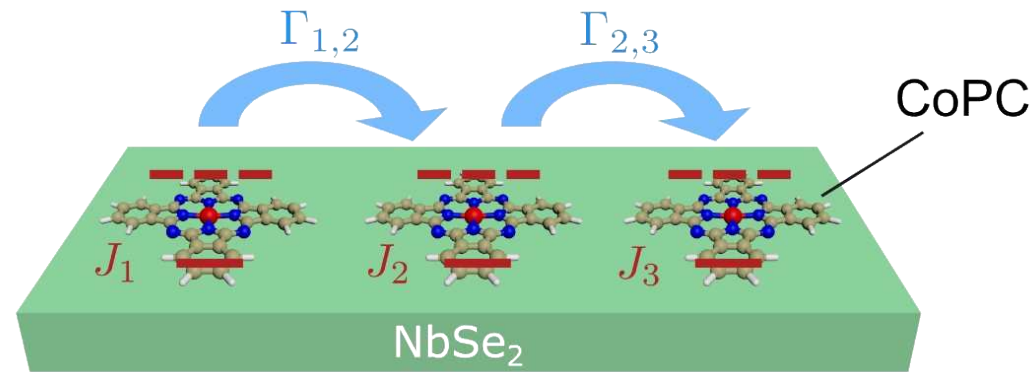


2D arrays have the largest width of the spin excitation

Coupled and uncoupled inelastic excitation

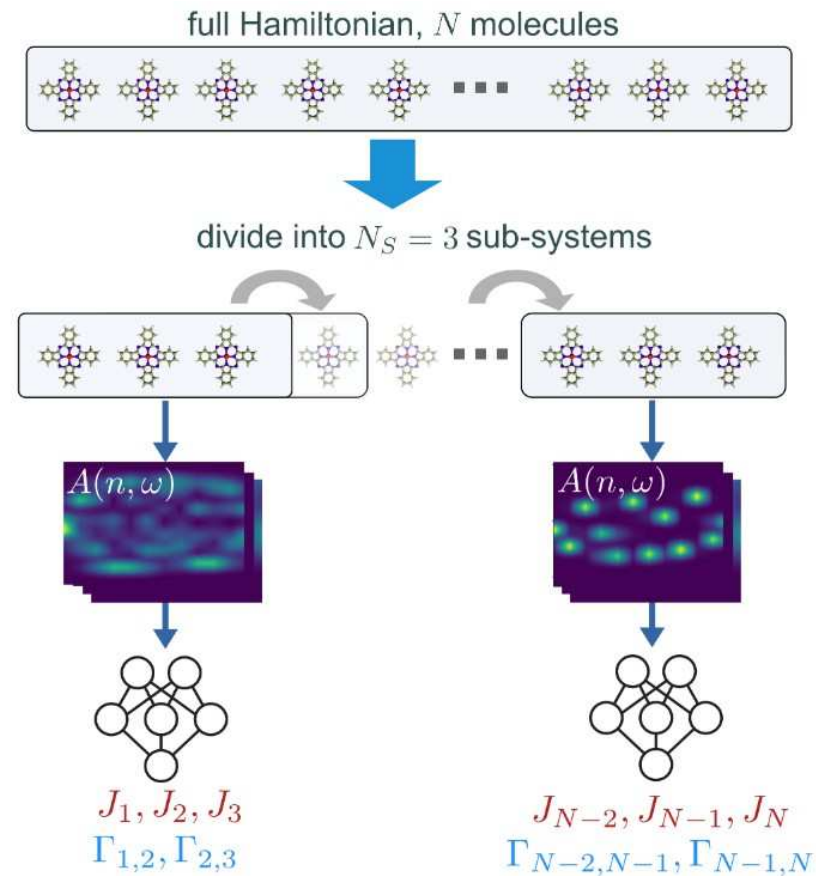


A strategy for machine learning quantum magnets



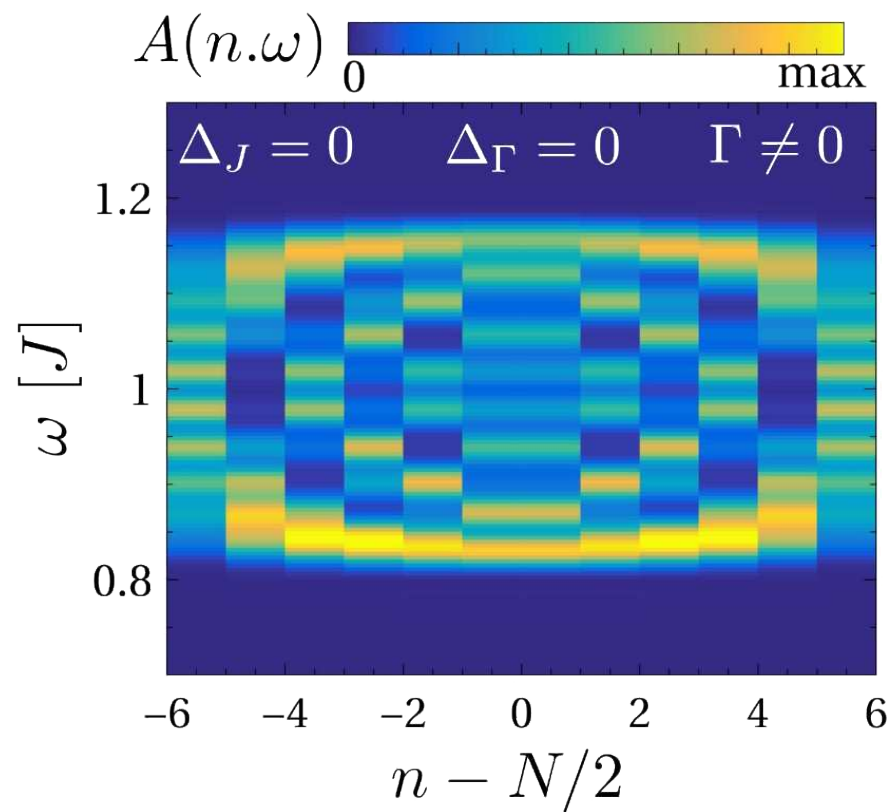
$\Gamma_{n,n+1}$: intermolecular exchange
 J_n : intramolecular exchange

$$H = \sum_n J_n \mathbf{S}_n \cdot \mathbf{K}_n + \sum_n \Gamma_{n,n+1} \mathbf{S}_n \cdot \mathbf{S}_{n+1}$$

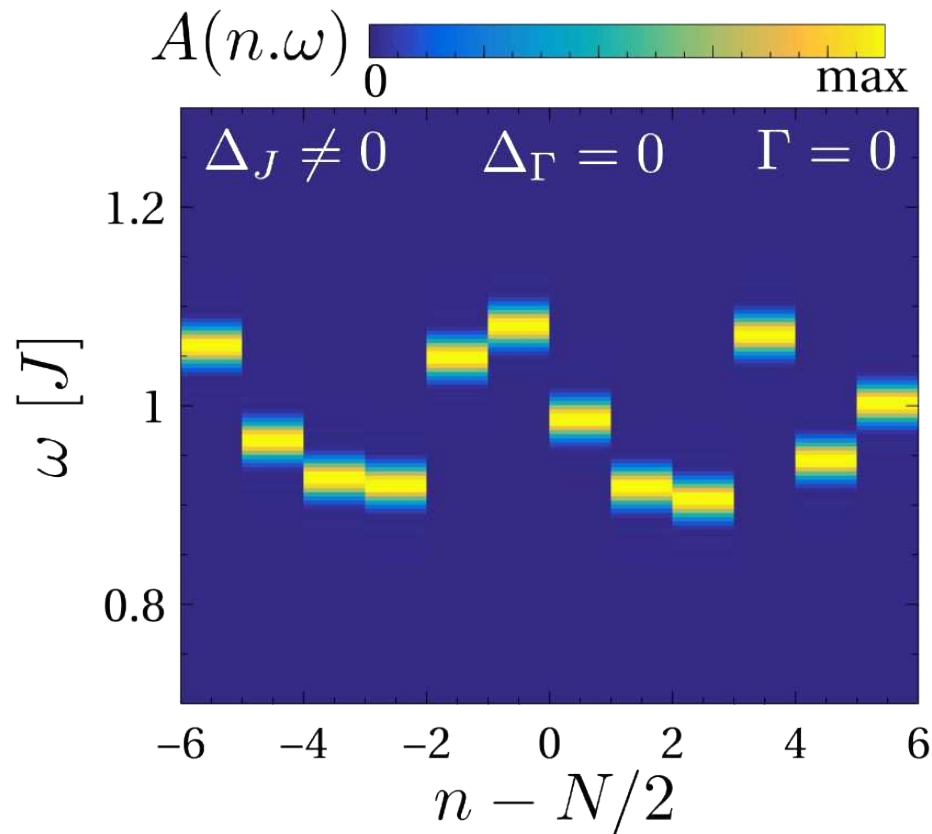


Pristine triplon excitations

Pristine and coupled molecules

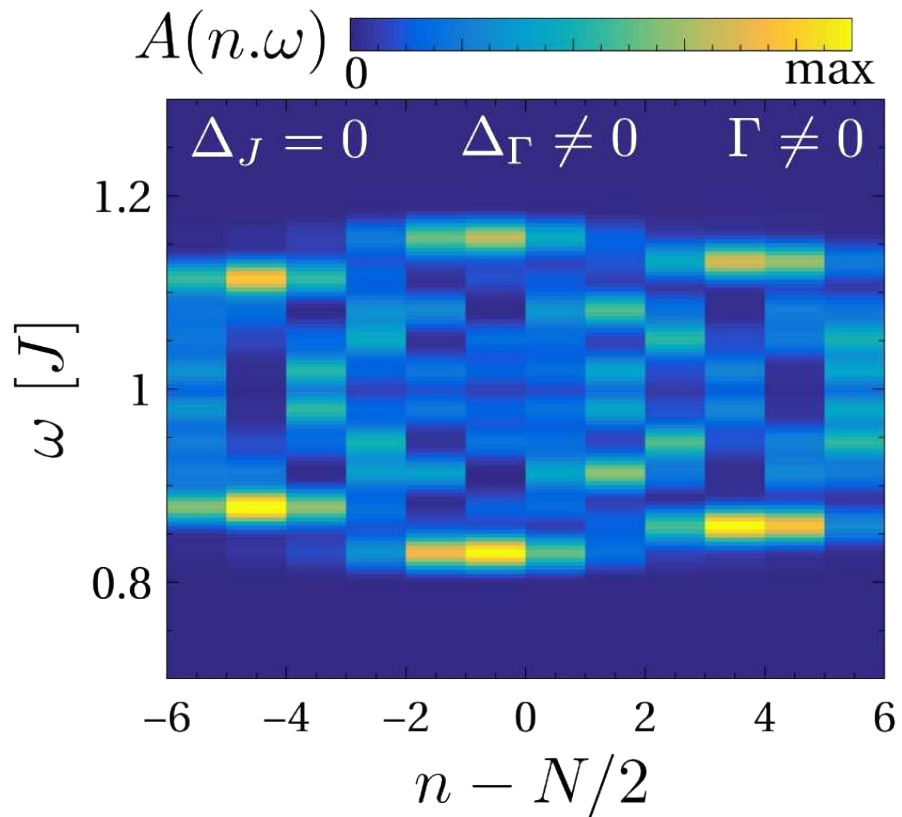


Decoupled and disordered molecules

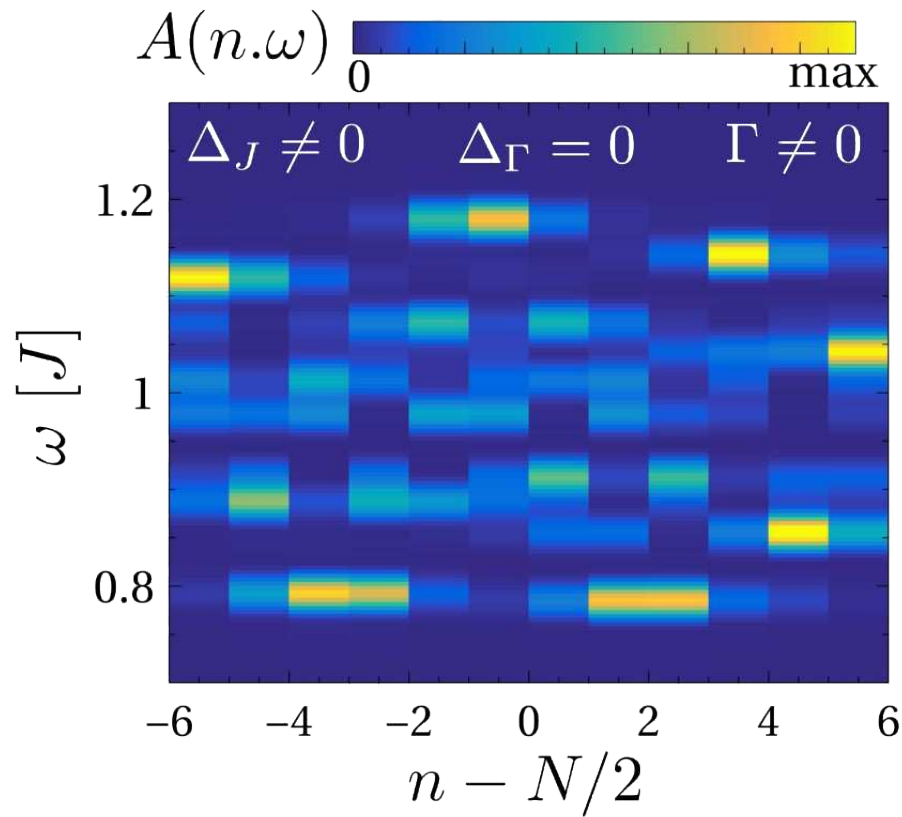


The different impact of molecular disorder

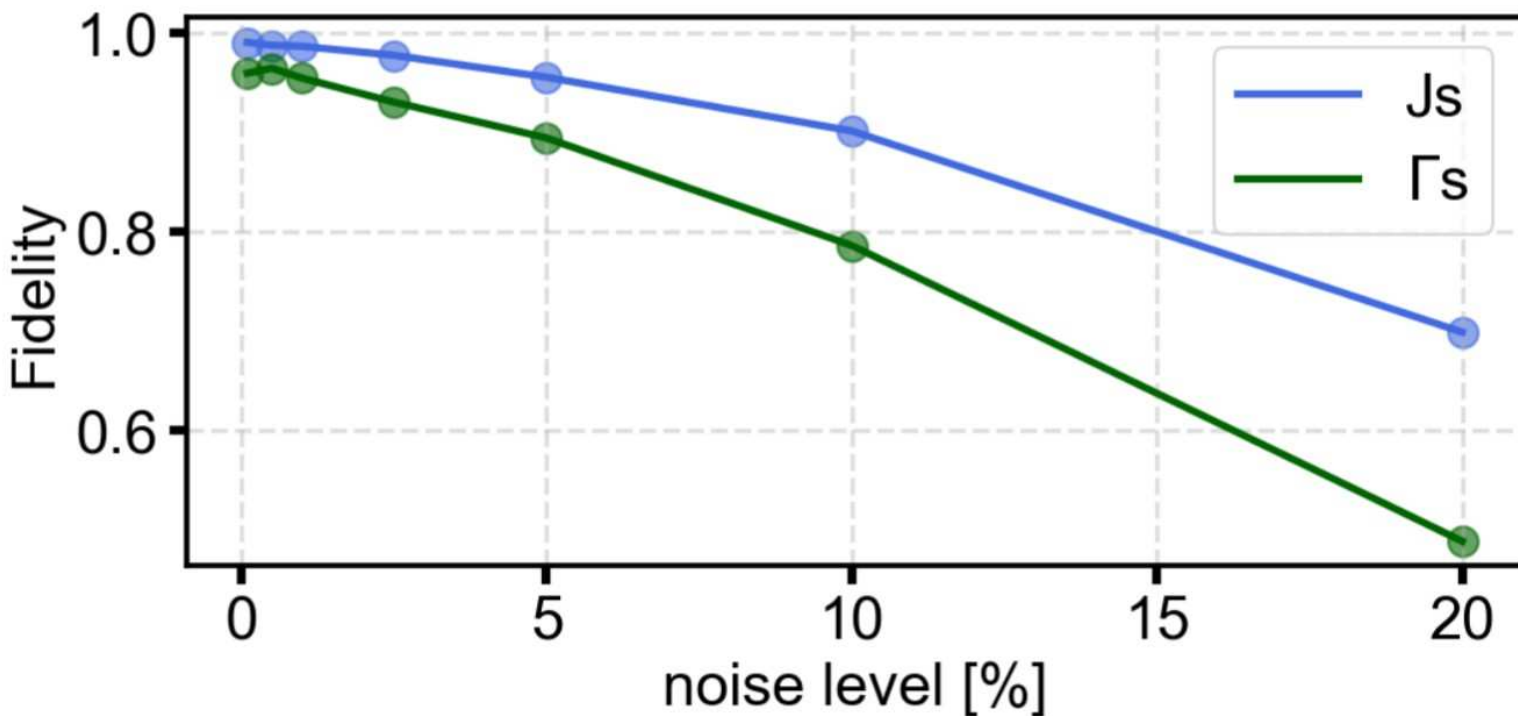
Disorder in inter-molecule coupling



Disorder in intra-molecule coupling

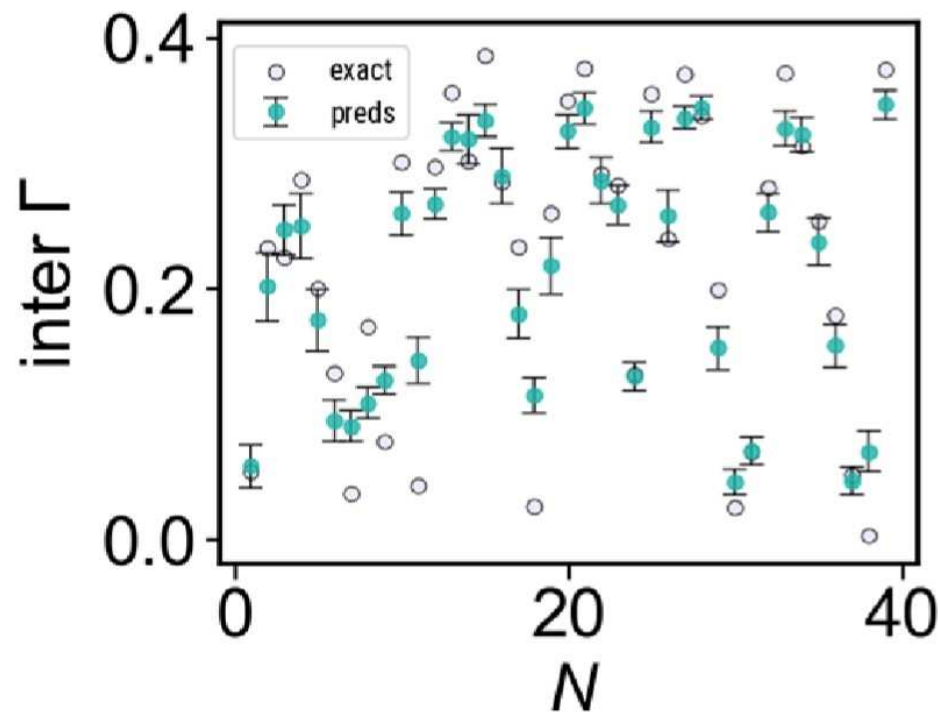
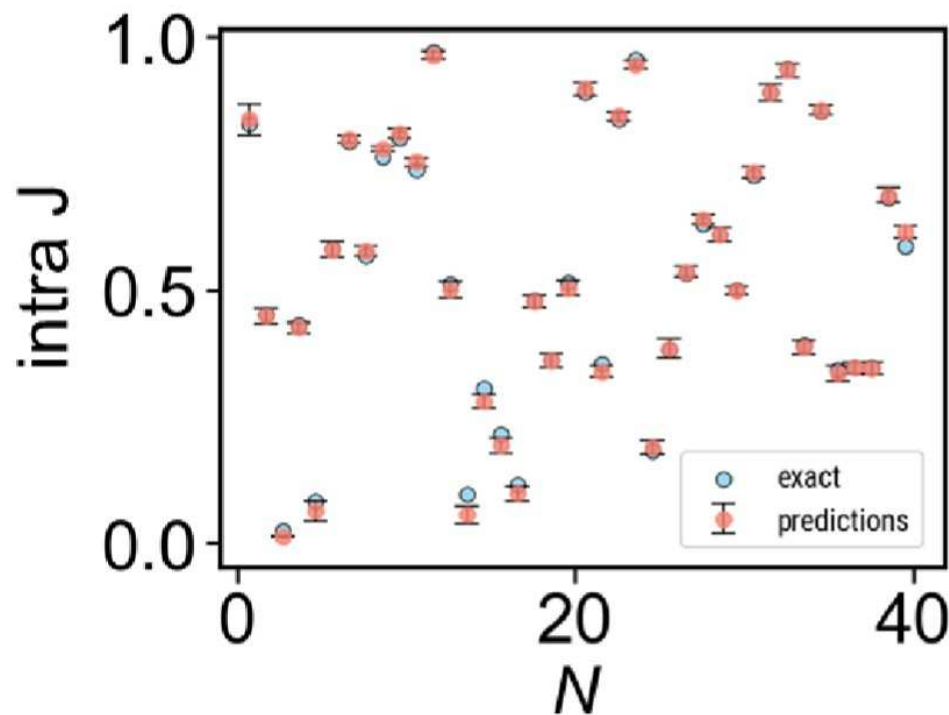


Resilience to noise of Hamiltonian learning



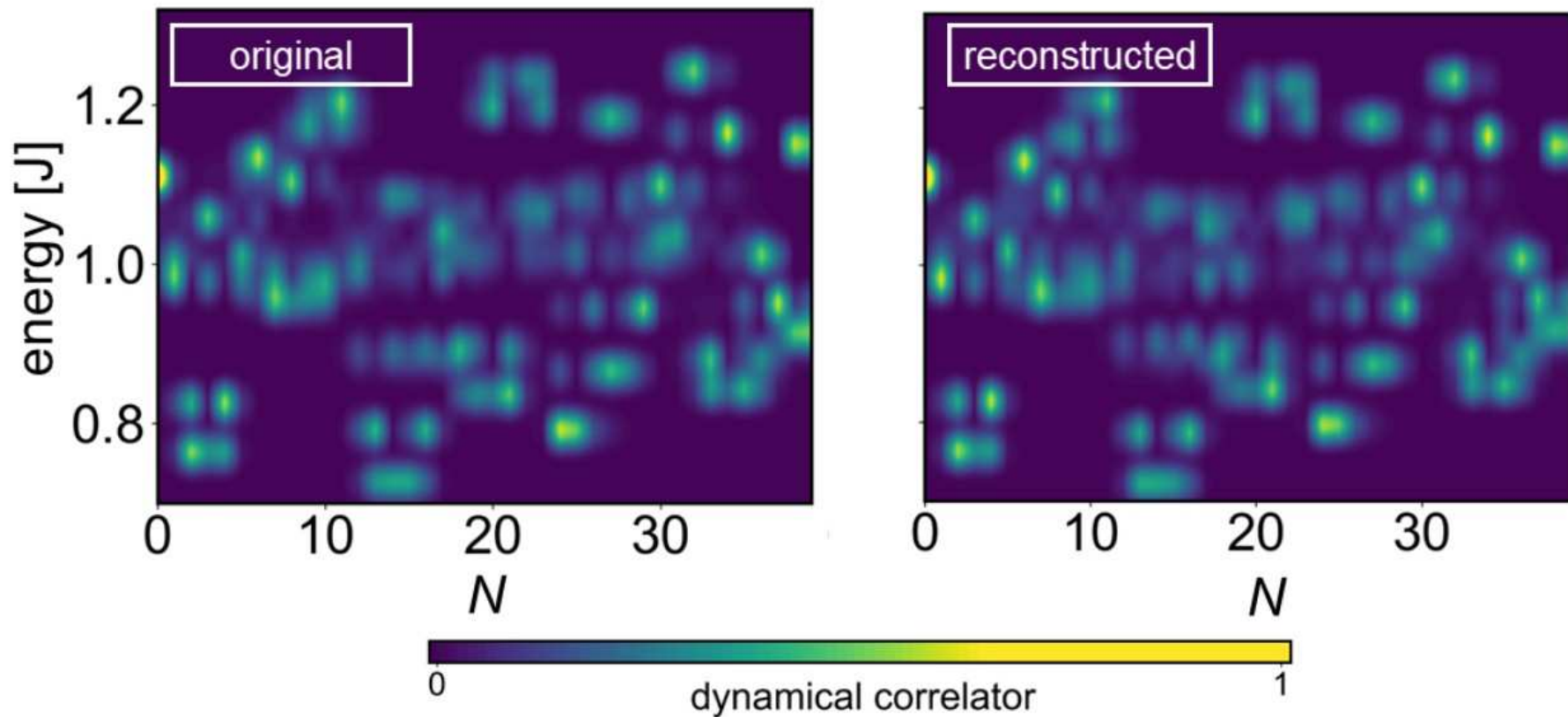
Noise model
$$\left(\frac{dI}{dV}\right)_{\text{noise}} = \left(\frac{dI}{dV}\right)_{\text{data}} + \eta \cdot \mathbf{R}$$

Inferring spatially dependent exchange couplings

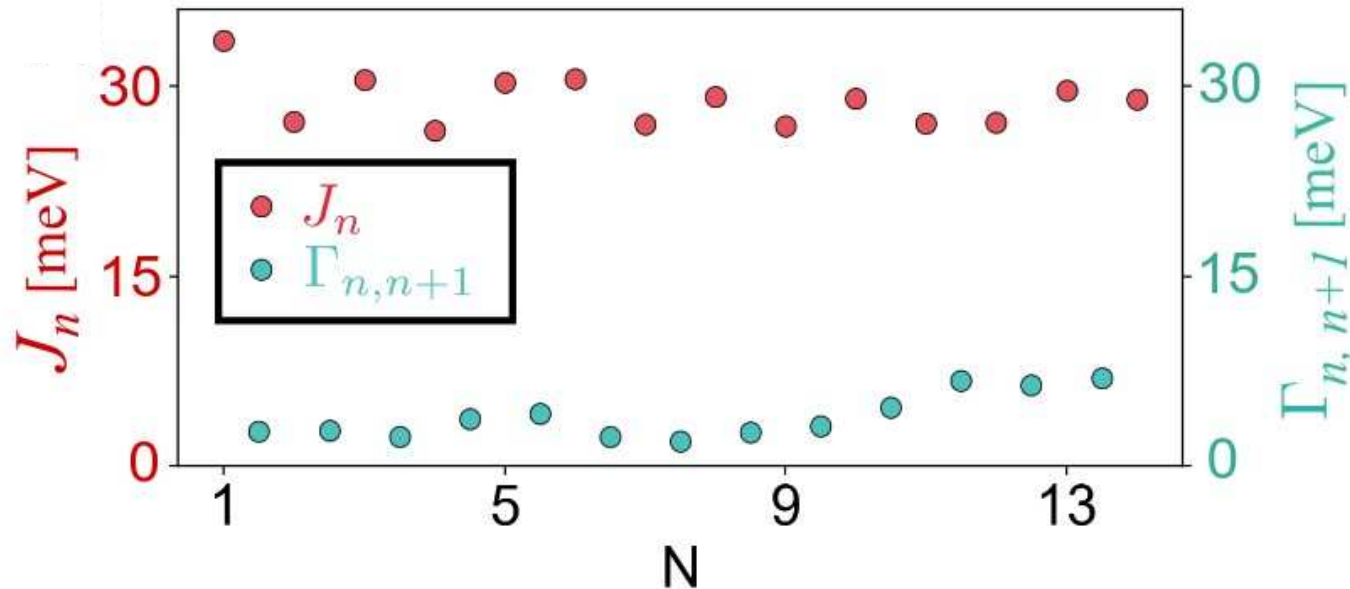


Intramolecular J_n exchange variations can be predicted robustly
Intermolecular Γ_n exchange variations are more subtle to predict

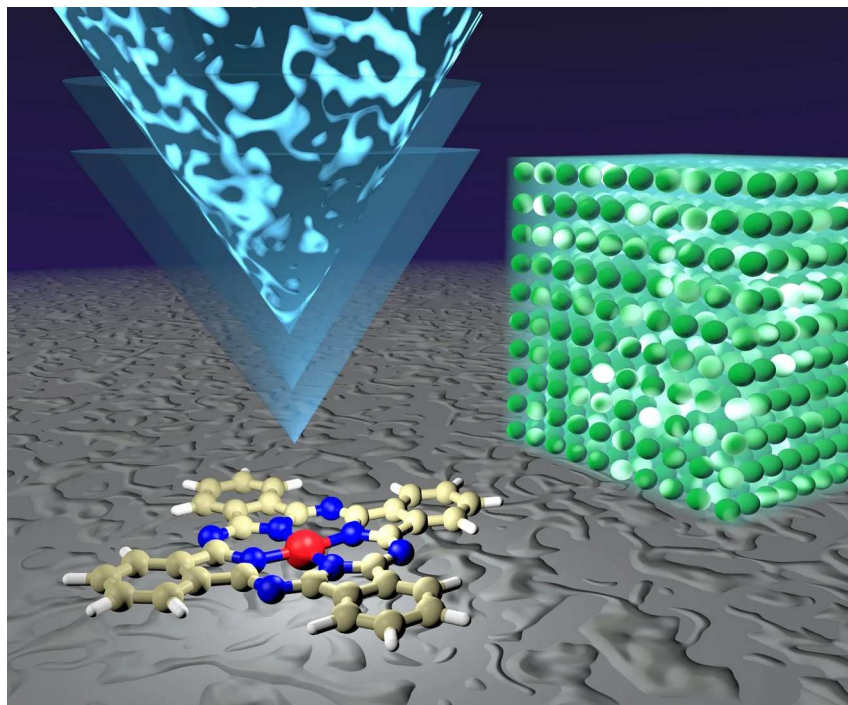
Reconstructing a quantum magnet Hamiltonian



Machine learning Hamiltonian of the experimental triplon chain



Hamiltonian learning from setpoint dependent spectroscopy



arXiv:2601.19371 (2026)

Greta Lupi



Mohammad Amini



Robert Drost



Adolfo Fumega

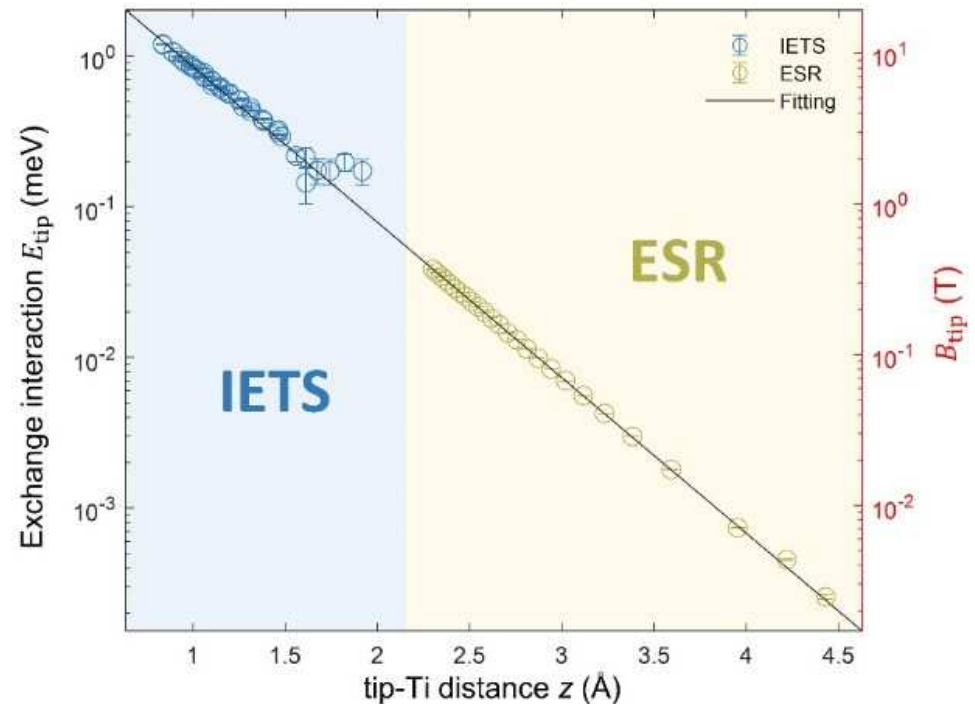
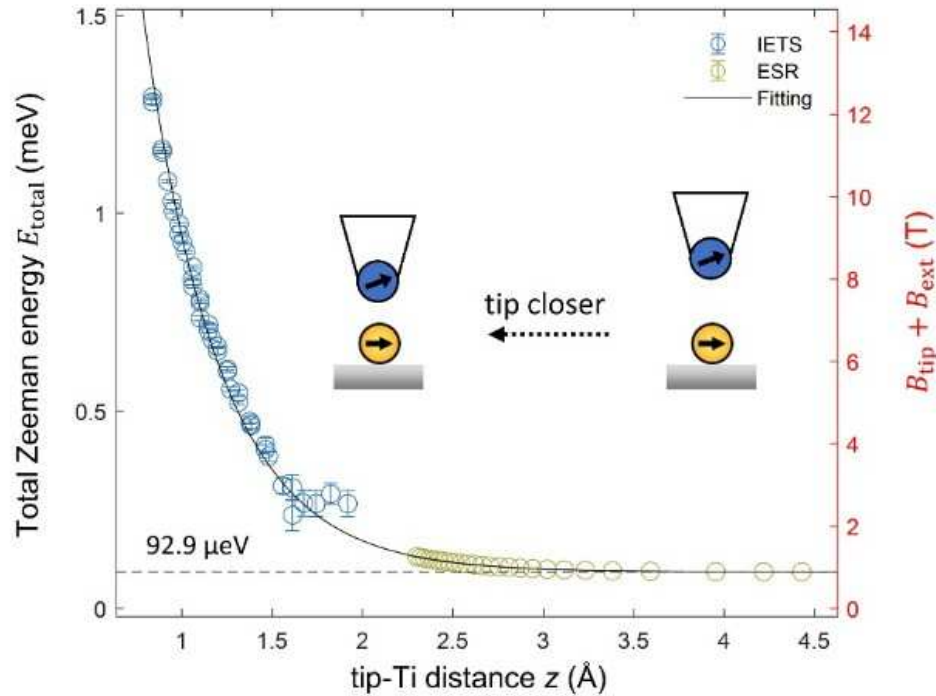


Peter Liljeroth

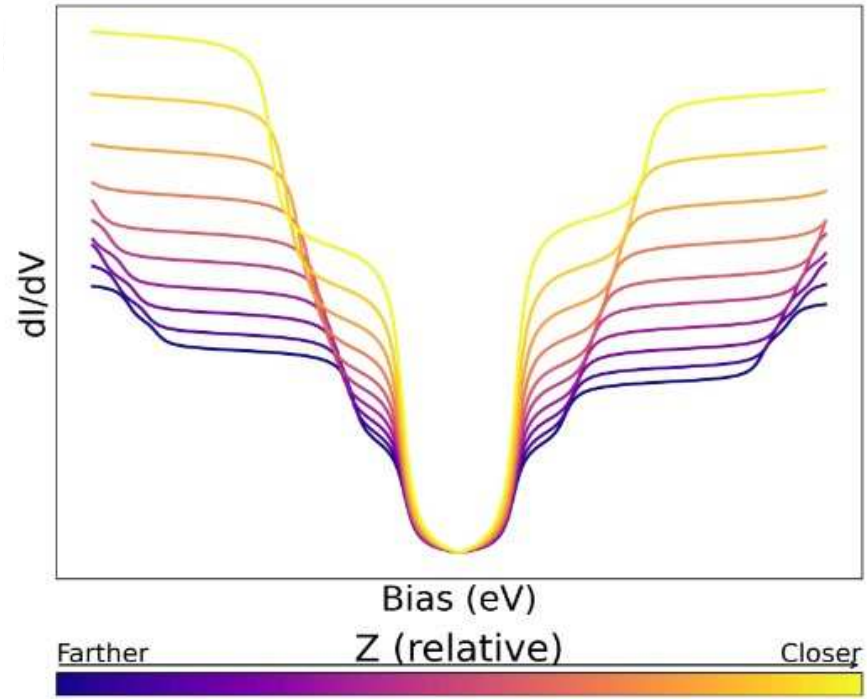
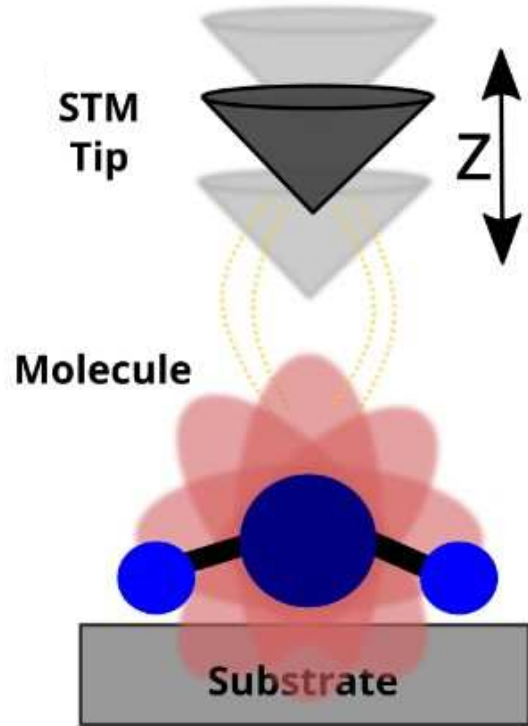


Many-body excitation energies can be distance dependent

The magnetic field of a spin-polarized STM tip affects the energy of the spin flip of a $S=1/2$

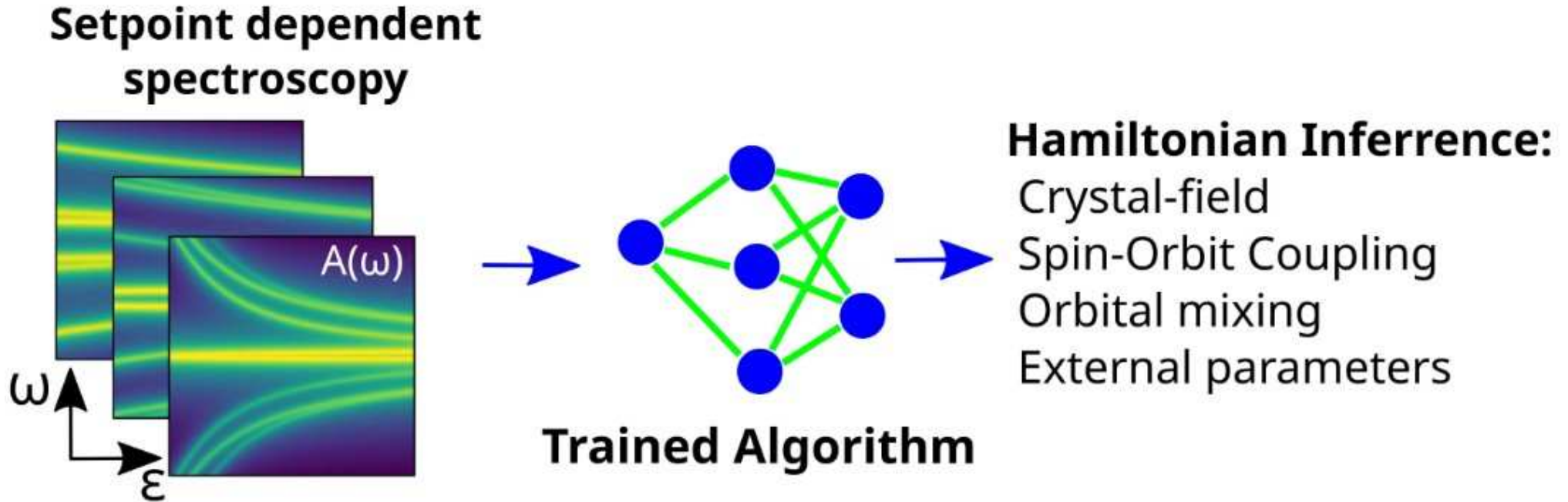


Distance-dependent spectroscopy in STM

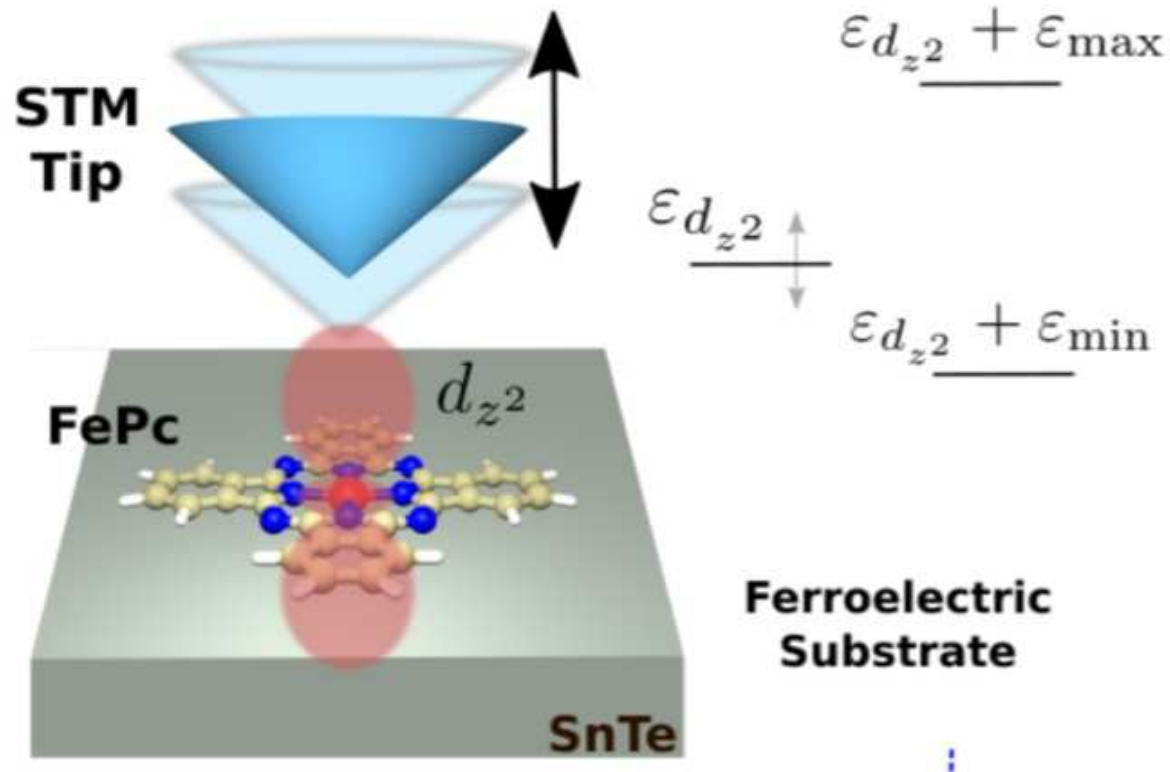


Spectroscopy can be distance dependent for specific systems
Can we learn the many-body Hamiltonian from this dependence?

Learning Hamiltonians from distance-dependent spectroscopy

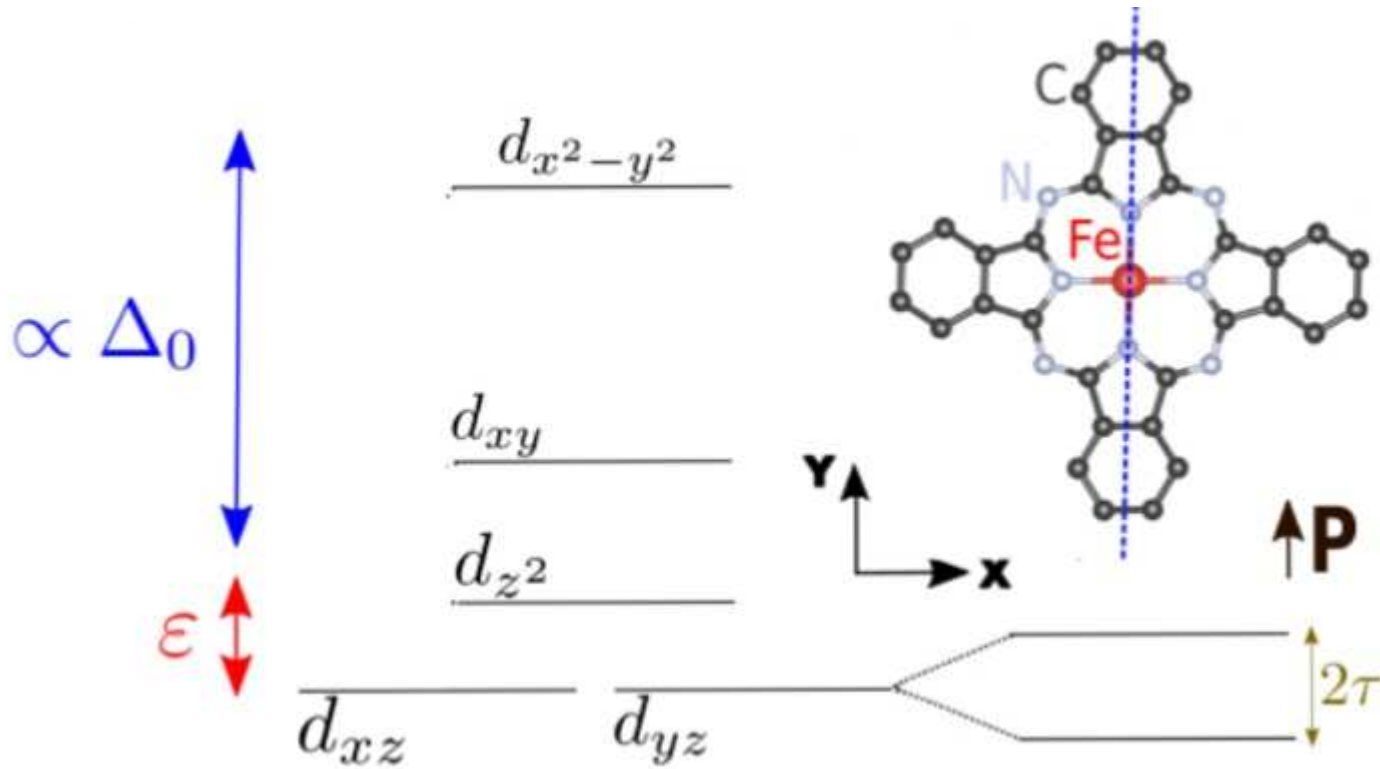


The impact of STM in a molecular many-body Hamiltonian



In a multiorbital system, the STM tip effectively impact different orbitals differently

Setpoint-dependent Hamiltonian



In a multiorbital system, the STM tip effectively impact different orbitals differently

Setpoint-dependent Hamiltonian

$$\mathcal{H} = \mathcal{H}_{\text{CF}}(z) + \mathcal{H}_{\text{Coulomb}} + \mathcal{H}_{\text{SOC}}$$

$$\mathcal{H}_{\text{CF}}(z) = \mathcal{H}_{\text{CF}}^0 + \mathcal{H}_{\text{CF}}^{\text{tip}}(z)$$

$$\mathcal{H}_{\text{CF}}^0 = \sum_{i,j,s} t_{ij} c_{i,s}^\dagger c_{j,s},$$

$$\mathcal{H}_{\text{Coulomb}} = \sum_{ijklss'} V_{ijkl} c_{i,s}^\dagger c_{k,s'}^\dagger c_{l,s'} c_{j,s}$$

$$\mathcal{H}_{\text{CF}}^{\text{tip}}(z) = \sum_{i,j,s} \gamma_{ij}(z) c_{i,s}^\dagger c_{j,s}$$

$$\mathcal{H}_{\text{SOC}} = \lambda_{\text{SOC}} \sum_{ij\alpha ss'} \ell_{ij}^\alpha \sigma_{ss'}^\alpha c_{i,s}^\dagger c_{j,s'},$$

Distance dependence



Setpoint-dependent inelastic excitations

Spin flip excitations

Orbital many-body excitations

Setpoint-dependent inelastic excitations

$$\mathcal{H} = \mathcal{H}_{\text{CF}}(z) + \mathcal{H}_{\text{Coulomb}} + \mathcal{H}_{\text{SOC}}$$

Spin-flip excitations

$$A_{\text{flip}}(\omega) = \sum_{\nu} \langle \Omega | \hat{S}_{d_{z^2}}^{\nu} \delta(\omega - \mathcal{H} + E_{\Omega}) \hat{S}_{d_{z^2}}^{\nu} | \Omega \rangle$$

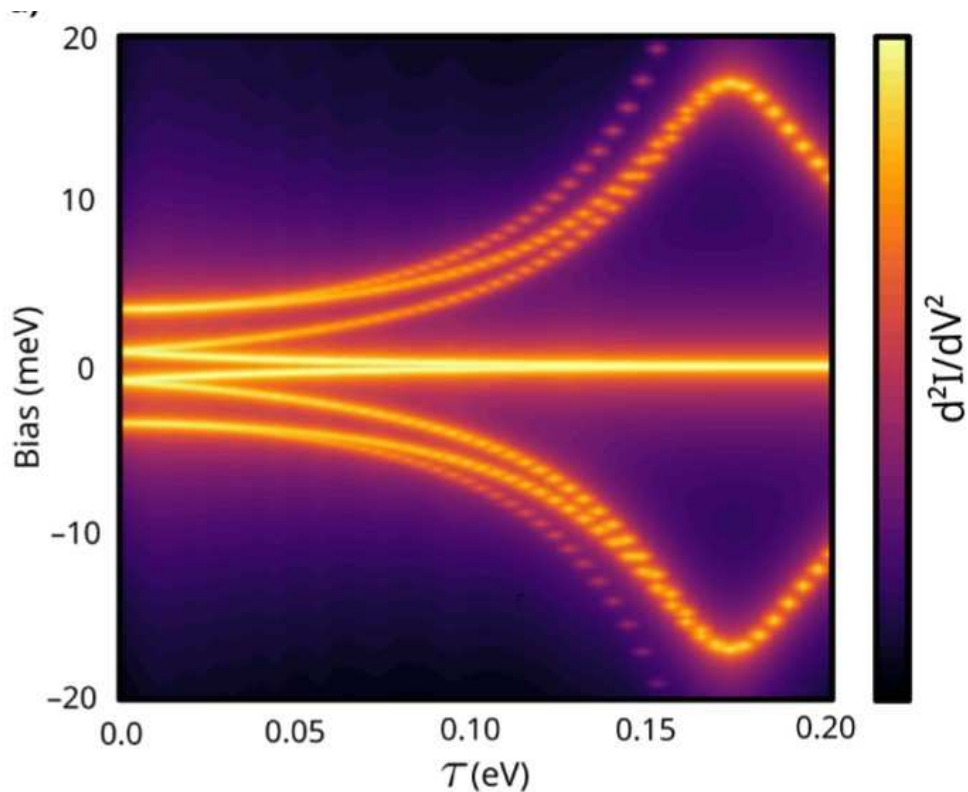
Orbital many-body excitations

$$A_{\text{orb}}(\omega) = \sum_{\alpha, s, s'} \Theta(\omega) C_{d_{z^2}, \alpha}^{s, s'}(\omega) + [1 - \Theta(\omega)] C_{\alpha, d_{z^2}}^{s, s'}(\omega)$$

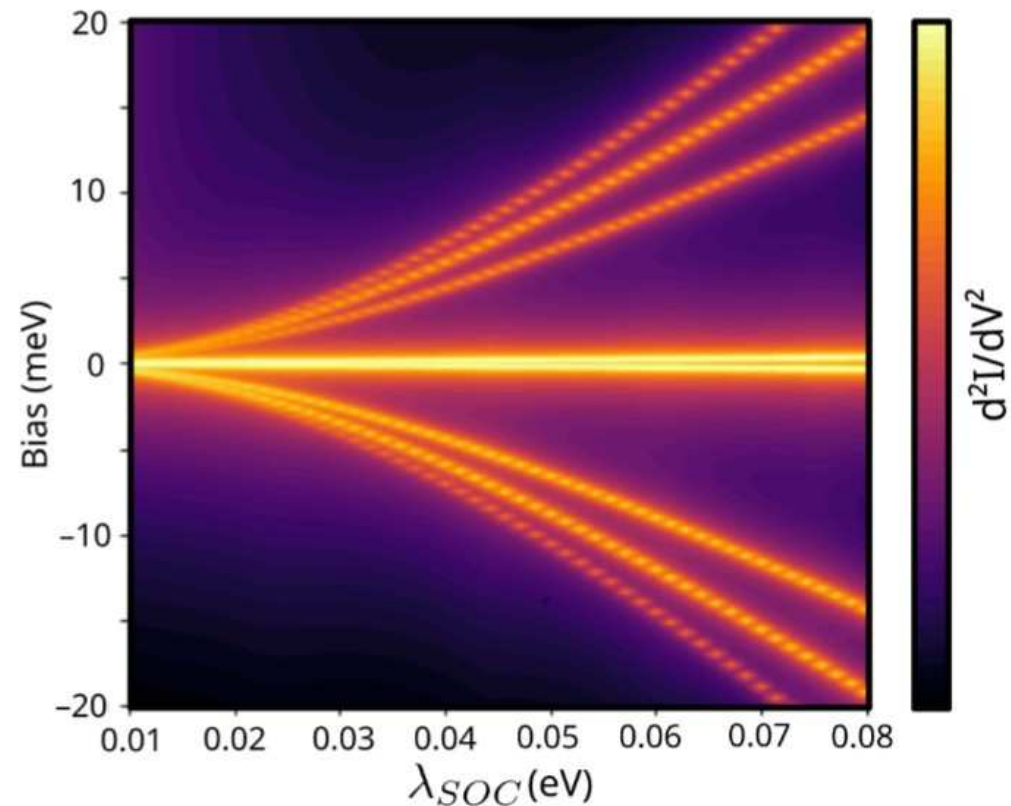
$$C_{\alpha, \beta}^{s, s'}(\omega) = \langle \Omega | c_{\beta, s}^{\dagger} c_{\alpha, s'} \delta(\omega - \mathcal{H} + E_{\Omega}) c_{\alpha, s'}^{\dagger} c_{\beta, s} | \Omega \rangle$$

Setpoint-dependent inelastic excitations

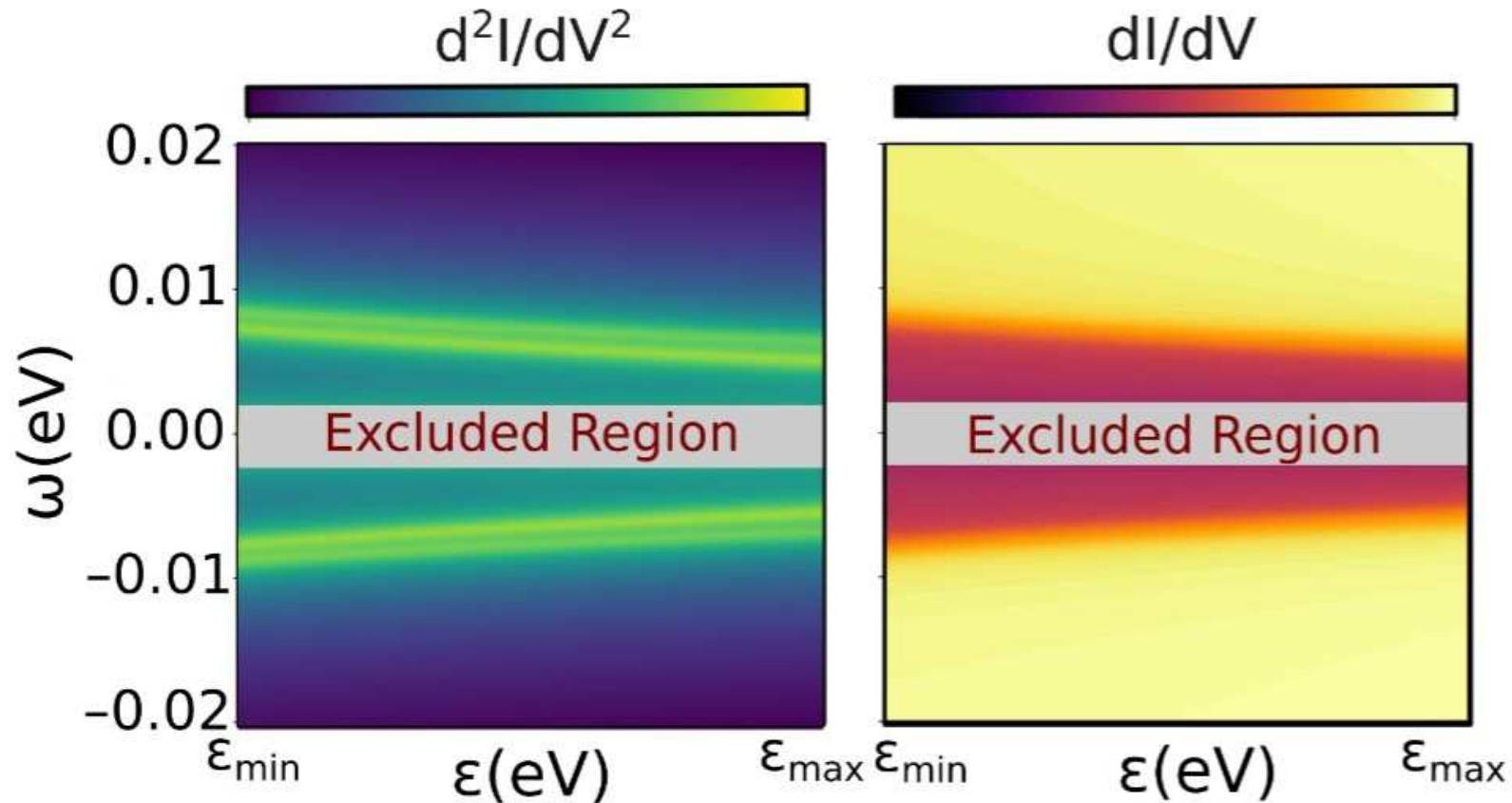
Dependence with crystal field



Dependence with spin-orbit coupling

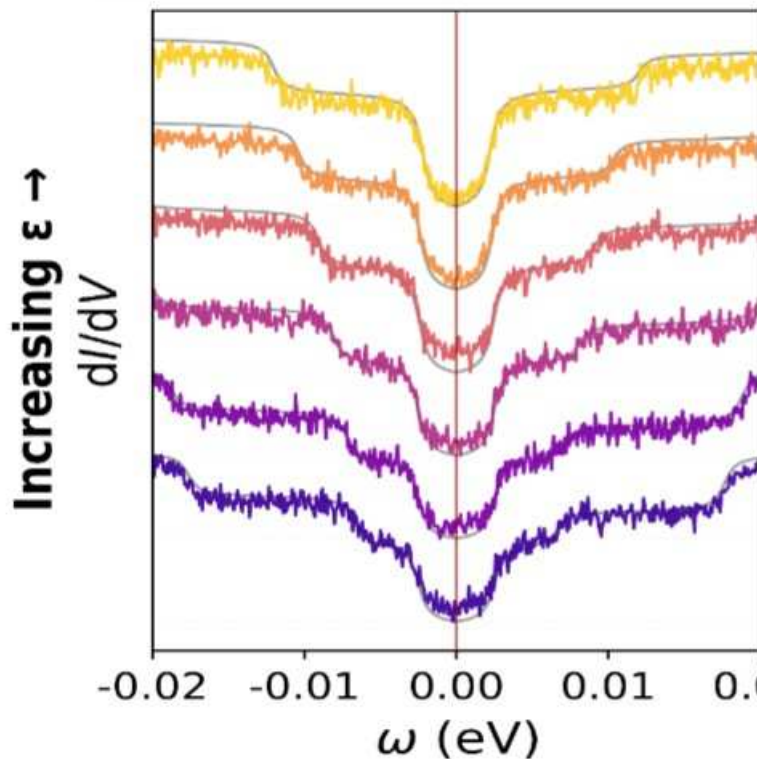


Inelastic spectroscopy of the molecular magnet

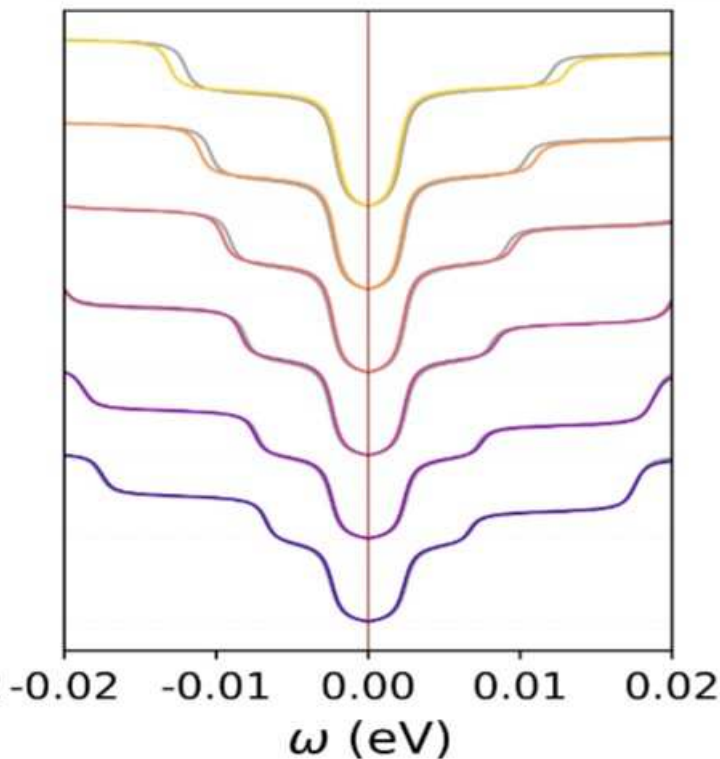


Original spectroscopy and learned Hamiltonian

Input spectroscopy



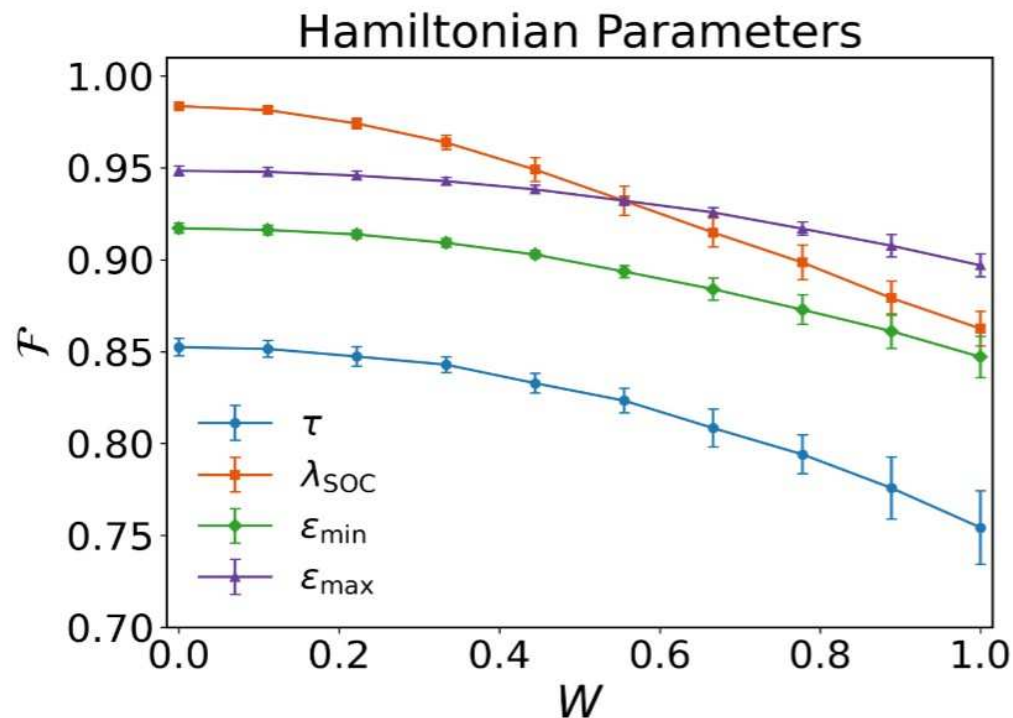
Spectroscopy of the learned Hamiltonian



Robustness of the Hamiltonian learning

Including noise

$$dI/dV_{\text{noisy}}(\varepsilon, \omega) = dI/dV_{\text{test}}(\varepsilon, \omega) + \chi_{\text{noise}}(\varepsilon, \omega)$$



$$\langle \chi_{\text{noise}}^2(\varepsilon, \omega) \rangle = W^2$$

Fidelity

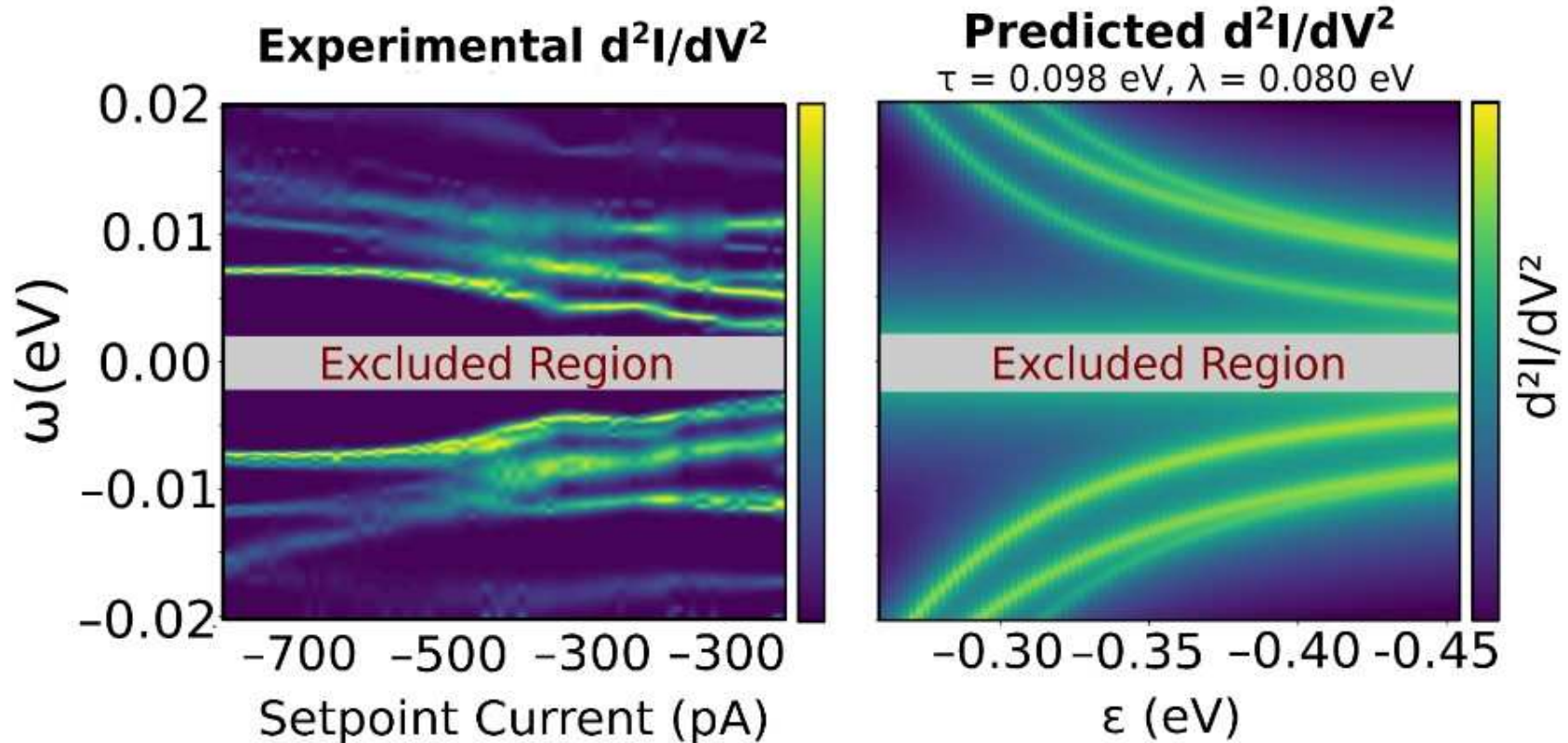
$$\mathcal{F} = 1$$

Perfect prediction

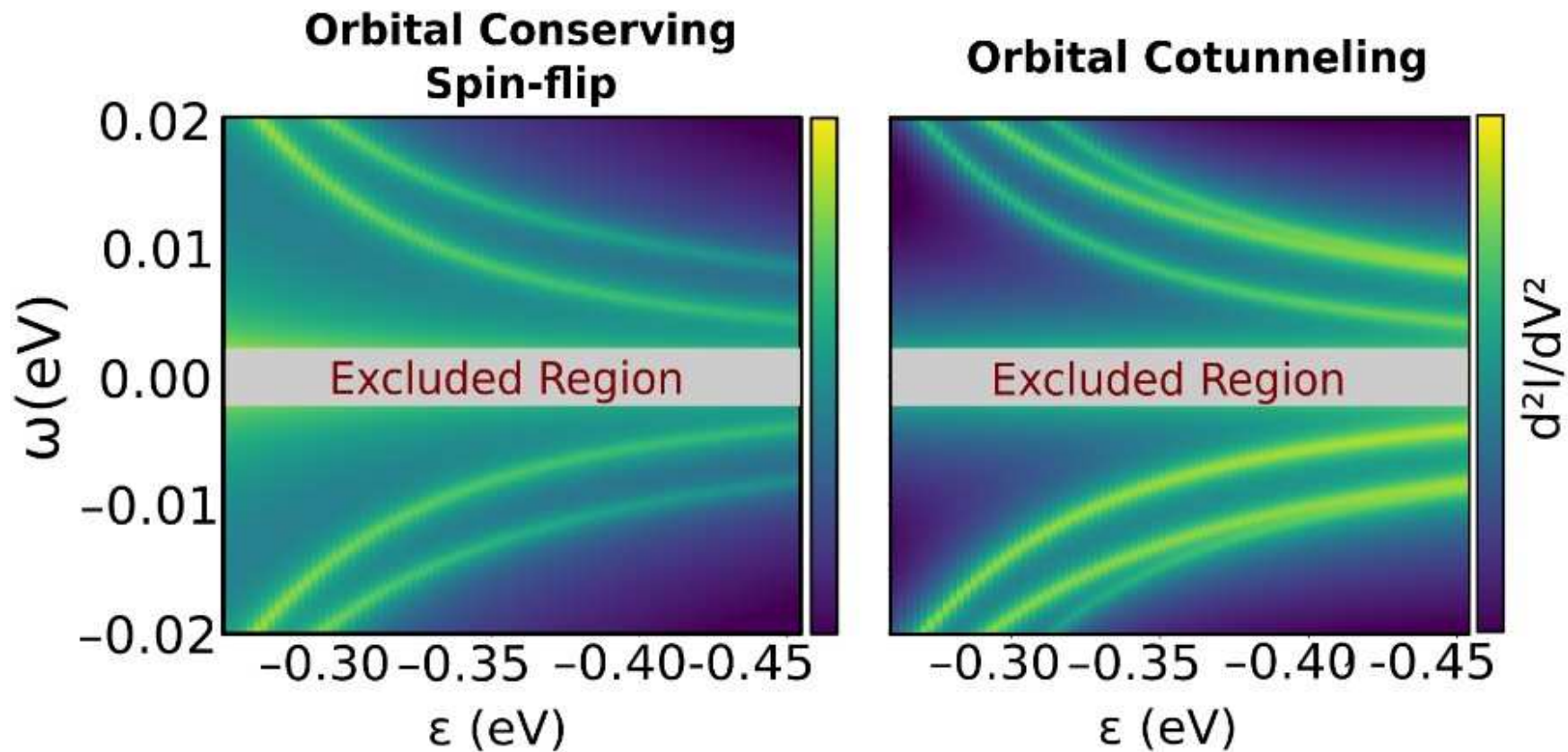
$$\mathcal{F} = 0$$

No prediction ability

Hamiltonian molecular learning from experimental spectroscopy



Disentangling inelastic channels



World of Quantum Materials

World of Quantum Materials

Travel the world of quantum materials, challenging other materials with quasiparticles

#	World	Course topic
1	The Mean Fields	Second quantization, mean-field, symmetry breaking
2	The Stone Lattice	Symmetries, tight-binding band structure
3	The Winding Borders	Topological band theory
4	The Storm Flats	Integer and fractional quantum Hall effect
5	The Vortex Glacier	Superconductivity, Nambu representation, Majoranas
6	The Broken Coast	Classical magnetism and magnons
7	The Entangled Web	Quantum entanglement and tensor networks
8	The Screened Swamp	Quantum magnetism, spinons, Kondo physics
9	The Defect Scars	Excitations and defects
10	The Devouring Mirror	Machine learning for quantum materials

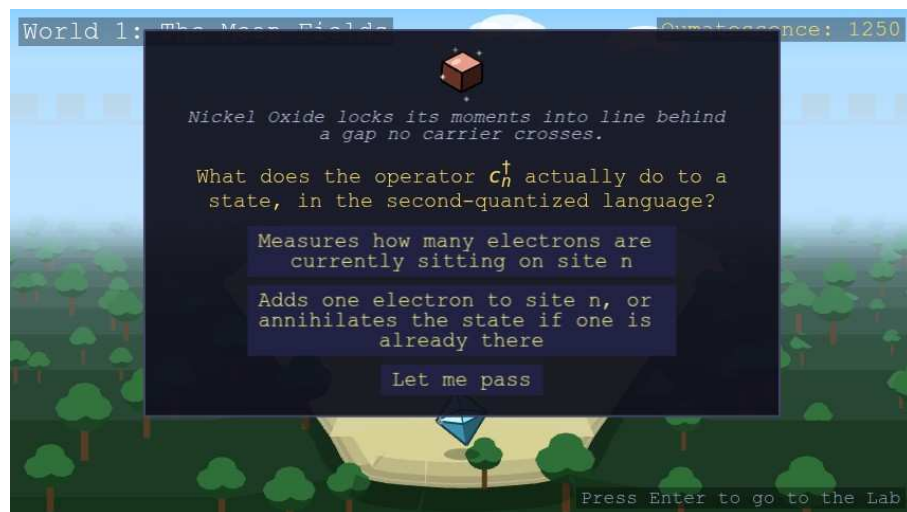


https://github.com/joselado/world_of_quantum_materials

Based on the Advanced Quantum Materials course at Aalto

World of Quantum Materials

Power-up answering quantum materials questions



Battle using quasiparticles



https://github.com/joselado/world_of_quantum_materials

Based on the Advanced Quantum Materials course at Aalto



*Nickel Oxide locks its moments into line behind
a gap no carrier crosses.*

Lithium fluoride (LiF) has a band gap of
about 14 eV. Drop the electron-electron
Coulomb repulsion from a model Hamiltonian
of it. What happens to the gap?

It closes, the way a Mott gap does
once U is switched off

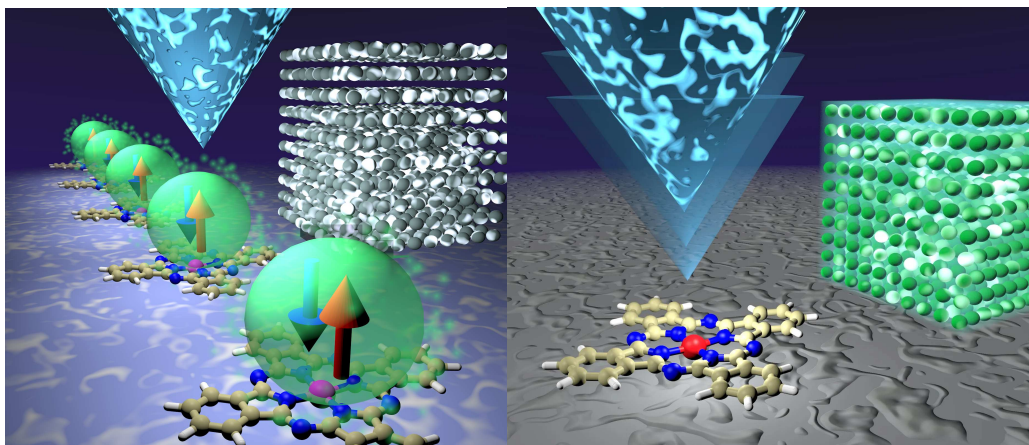
It stays open: a conventional
insulator's gap needs no repulsion

Let me pass



Take home

STM spectroscopy allows learning the Hamiltonian of complex collective quantum magnets, by leveraging machine learning trained with quantum many-body methods



Nano Letters 25, 36, 13435-13440 (2025)
arXiv:2601.19371 (2026)

Funding from

Finnish Quantum Flagship

