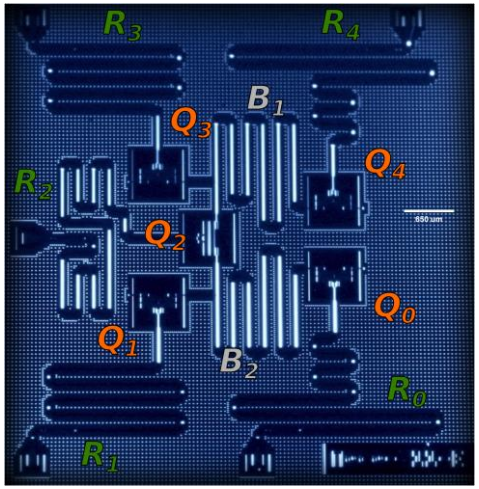
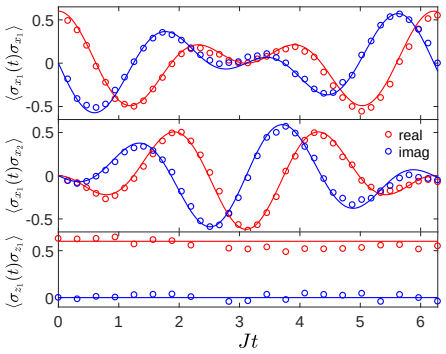
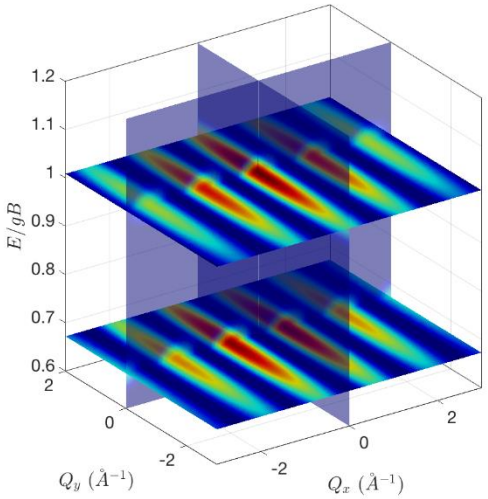






Quantum Simulation of spin models on IBM Quantum Computers

Stefano Carretta

Dipartimento di Scienze Matematiche, Fisiche e Informatiche

MOLECULAR MAGNETISM group

UNIVERSITÀ DI PARMA

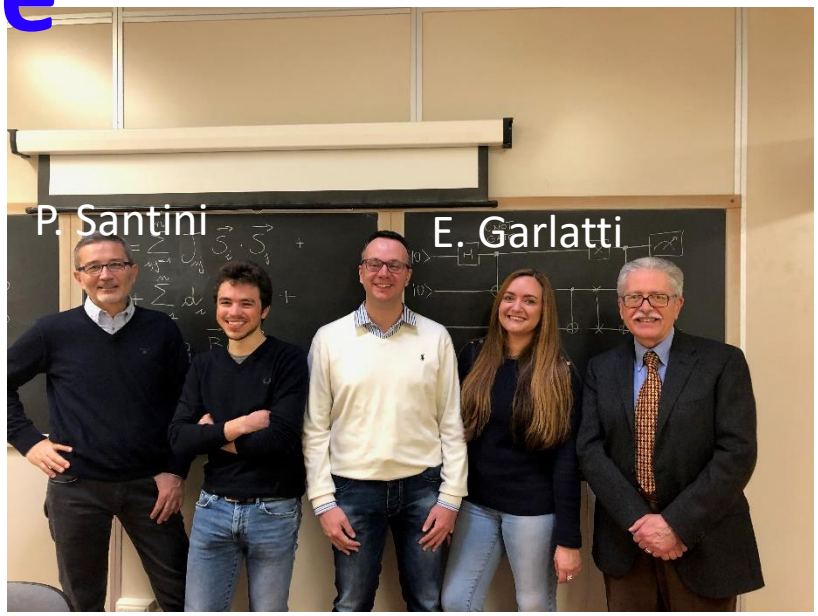
QIS.UNIPR.IT
QUANTUM INFORMATION SCIENCE @ UNIPR

People

UNIVERSITÀ DI PARMA

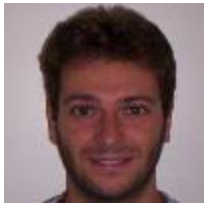
MOLECULAR MAGNETISM group

QIS.UNIPR.IT
QUANTUM INFORMATION SCIENCE @ UNIPR



A. Chiesa G. Amoretti

F. Tacchino



D. Gerace

IBM

I. Tavernelli

M. Grossi

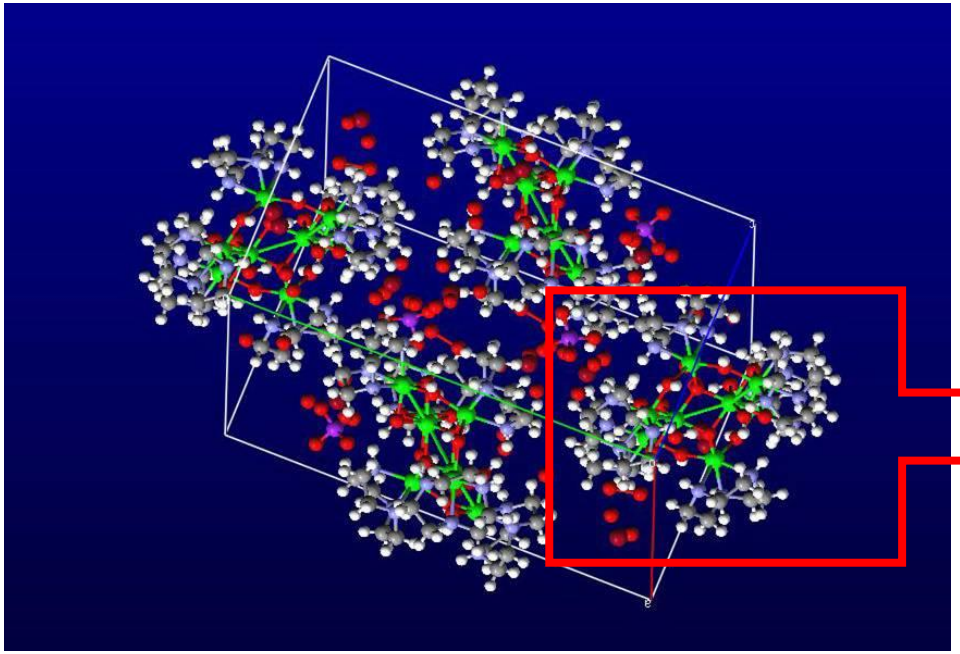
QUANTERA

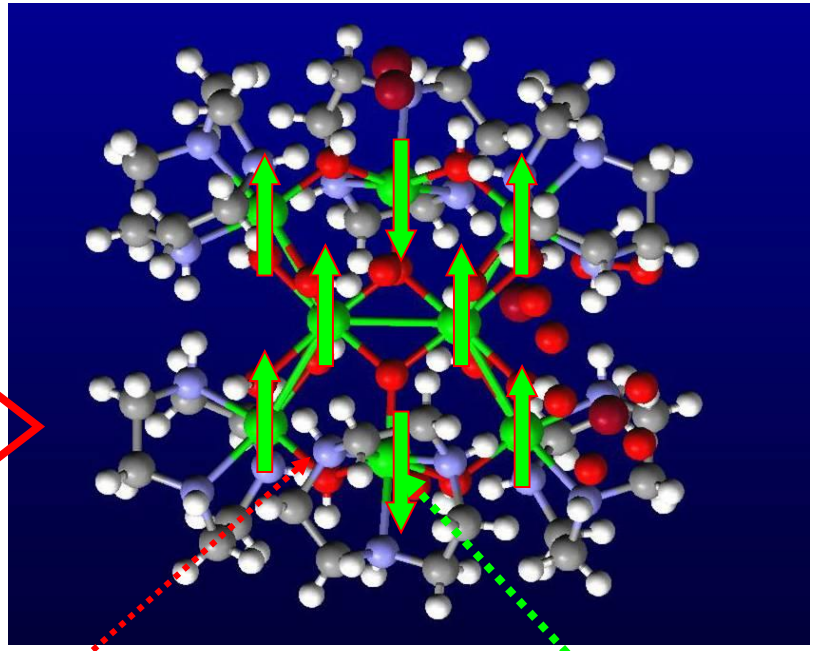
NUOVO BANDO PRIN
Progetti di ricerca di Rilevante Interesse Nazionale

UNIVERSITÀ DI PARMA

Molecular Nanomagnets

Each molecule contains a small number of exchange-coupled magnetic ions (spins). Molecules are arranged on a crystal lattice.



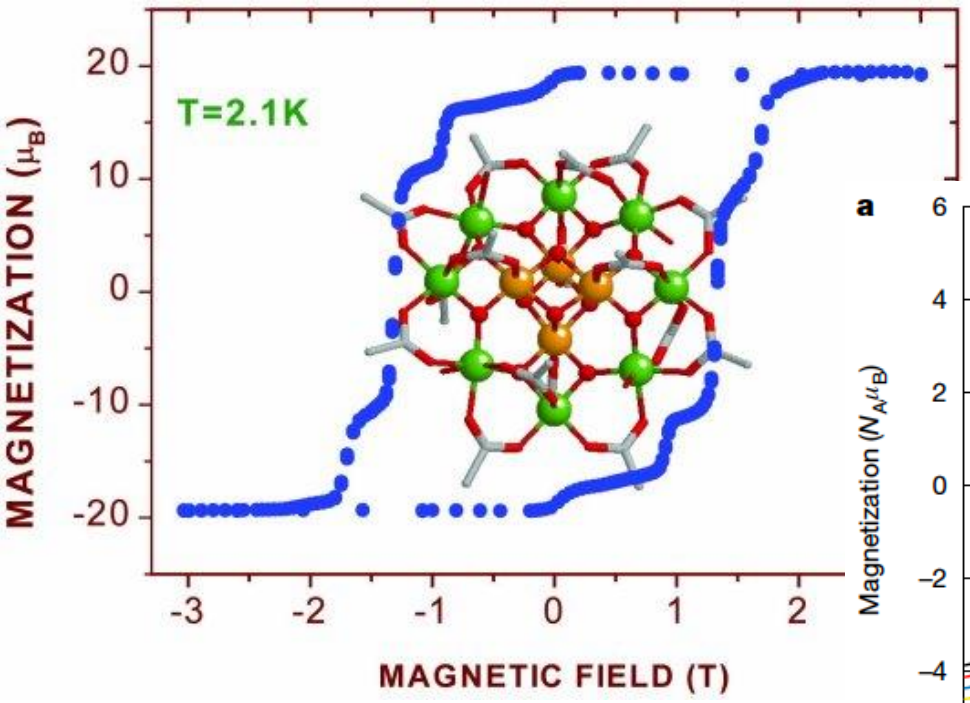


$Fe_8O_2(OH)_{12}(tacn)_6]Br_8$

Prototypical systems to study **quantum effects and promising for applications**

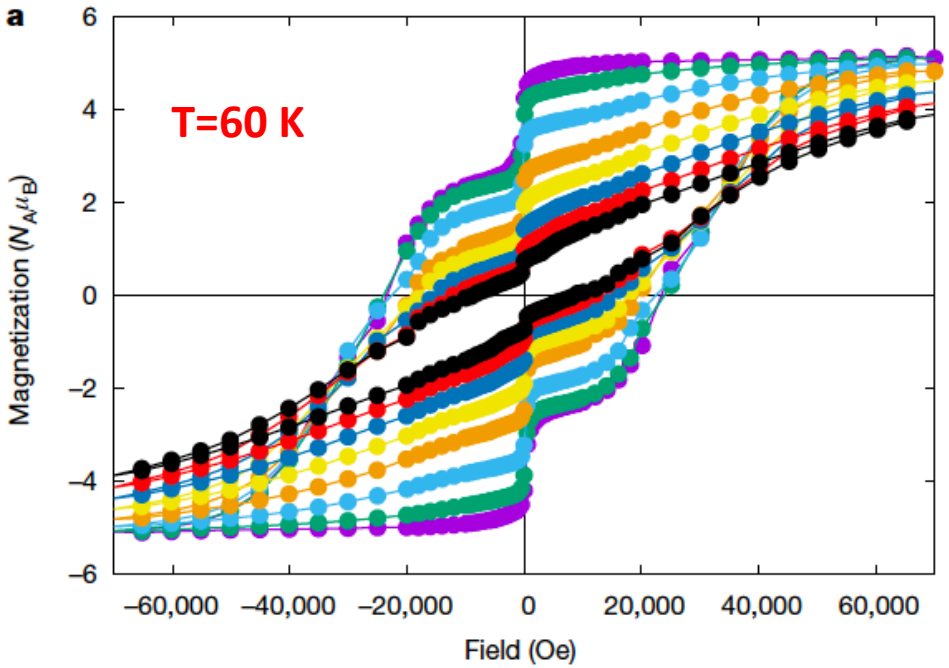
Molecular Nanomagnets as bits

Mn_{12}



Nature **365**, 141 (1993)

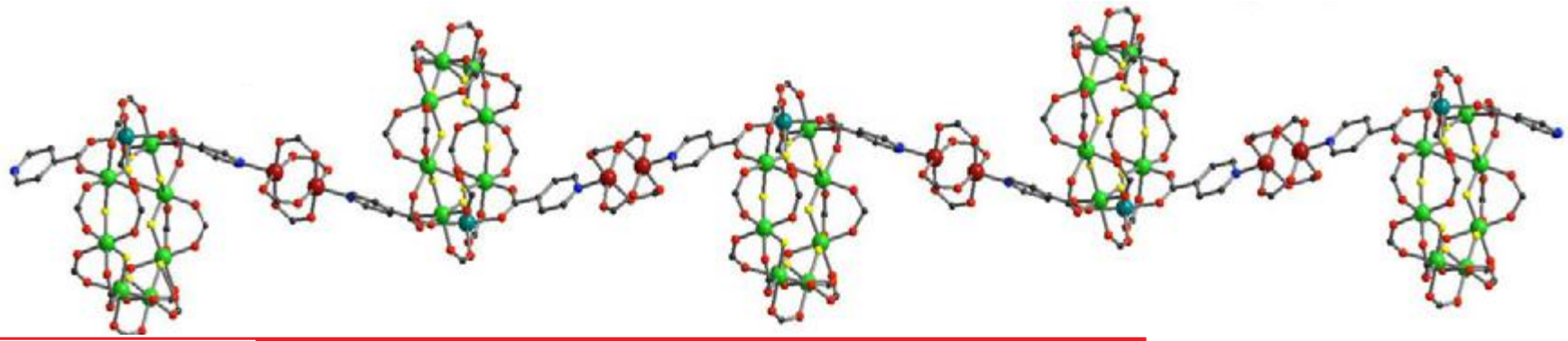
Dy-cene



Nature **548**, 439 (2017)

Hysteresis and **bistability** at the single-molecule level→ information storage in single molecules

Molecular Nanomagnets as qubits



nature nanotechnology

ARTICLES

CORRECTED ONLINE: 17 FEBRUARY 2009
PUBLISHED ONLINE: 1 FEBRUARY 2009 | DOI: 10.1038/NNANO.2008.404

Engineering the coupling between molecular spin qubits by coordination chemistry

Grigore A. Timco[1], Stefano Carretta[2], Fili
Christopher A. Muryn[1], Eric J. L. McInnes
Giuseppe Amoretti[2], Marco Affronte[3,4]*

nature COMMUNICATIONS

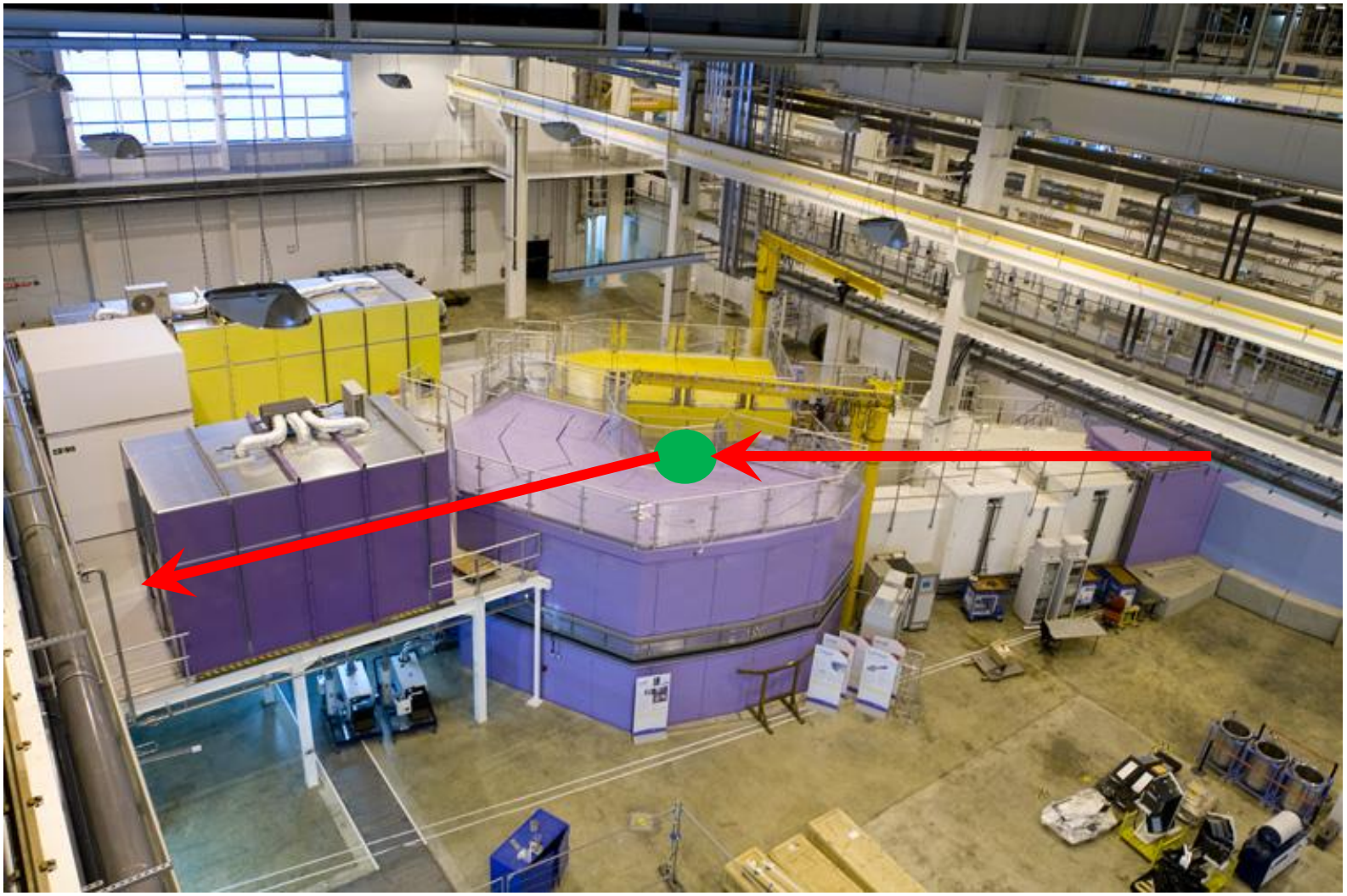
ARTICLE

Received 14 Aug 2015 | Accepted 21 Mar 2016 | Published 25 Apr 2016

DOI: 10.1038/ncomms11377 OPEN

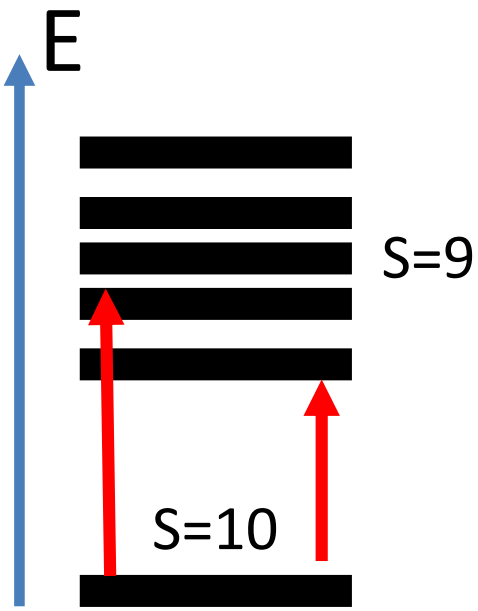
A modular design of molecular qubits to implement universal quantum gates

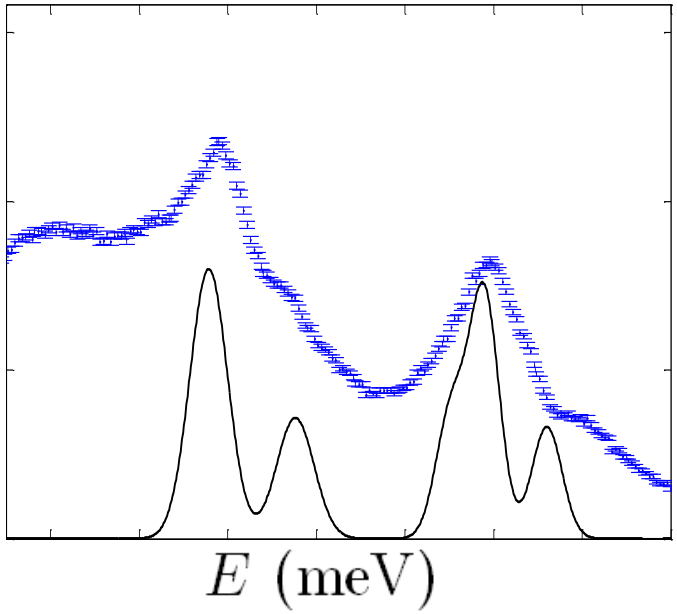
Inelastic Neutron Scattering



A lot of information can be obtained by studying how neutrons change their velocity when they are scattered by these materials.

Inelastic Neutron Scattering



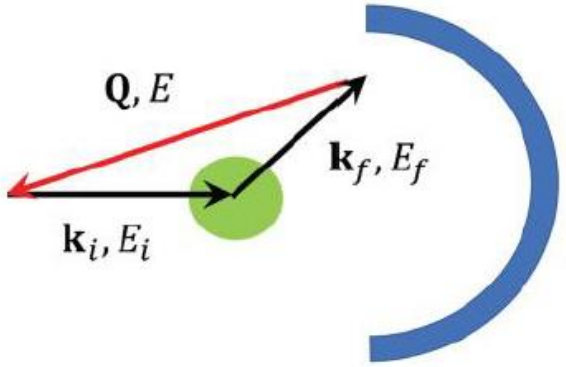


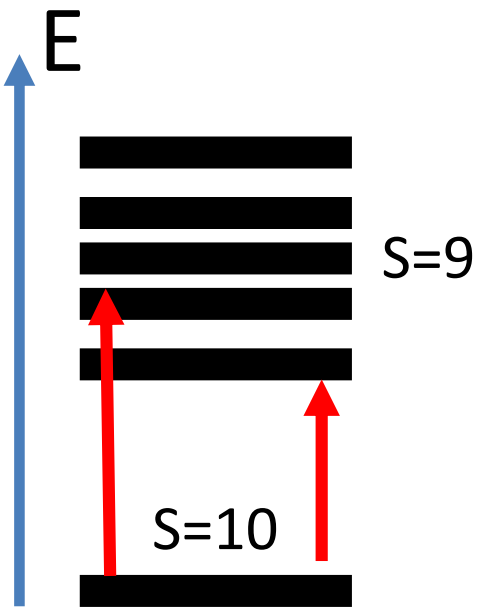
A lot of information can be obtained by studying how neutrons change their velocity when they are scattered by these materials.

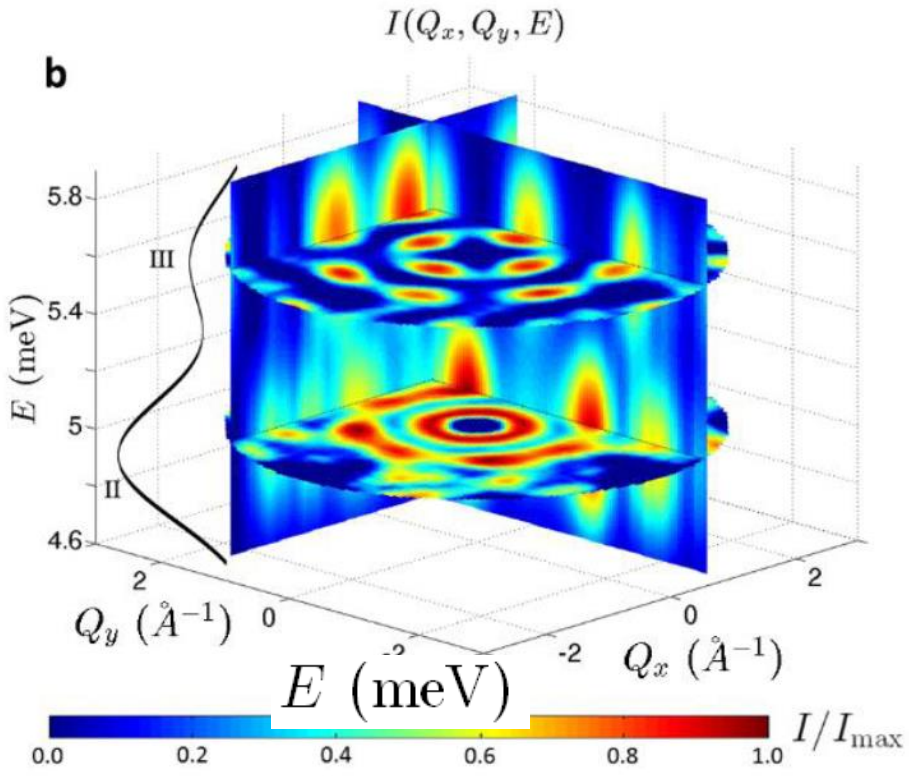
PRL 119, 217202 (2017)

Inelastic Neutron Scattering

The pattern of maxima and minima reflects the spatial structure of the states involved in the transition





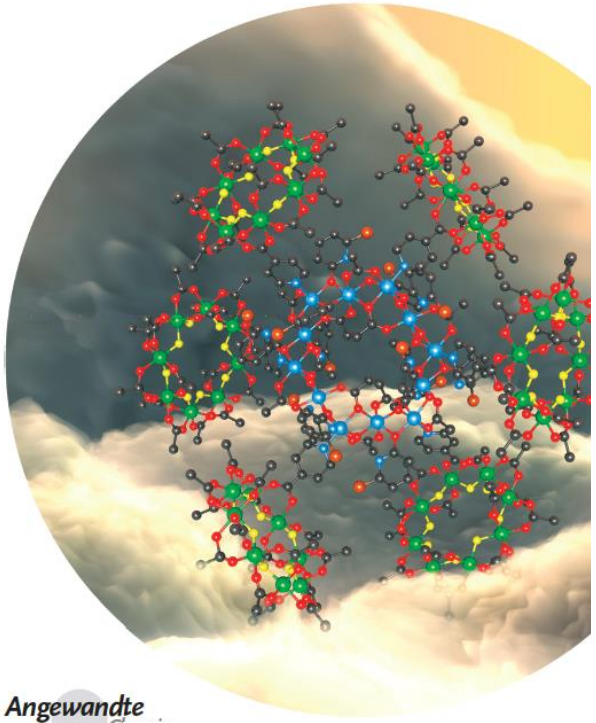


A lot of information can be obtained by studying how neutrons change their velocity when they are scattered by these materials.

PRL 119, 217202 (2017)

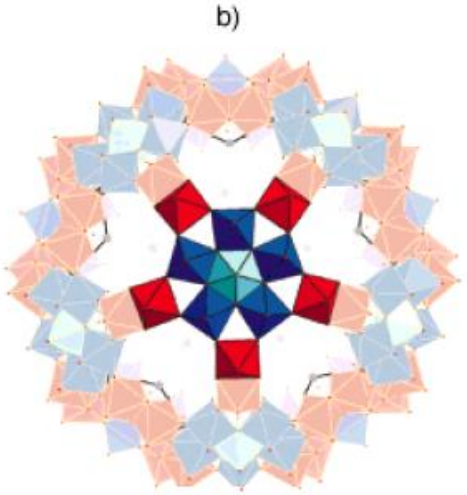
Challenge: interpretation of spectra of interesting molecules

- Experiments on rather small molecules can be interpreted by quantum simulations preformed on classical computers.
- However, there is an exponential increase of the required computational resources and many molecules cannot be understood.

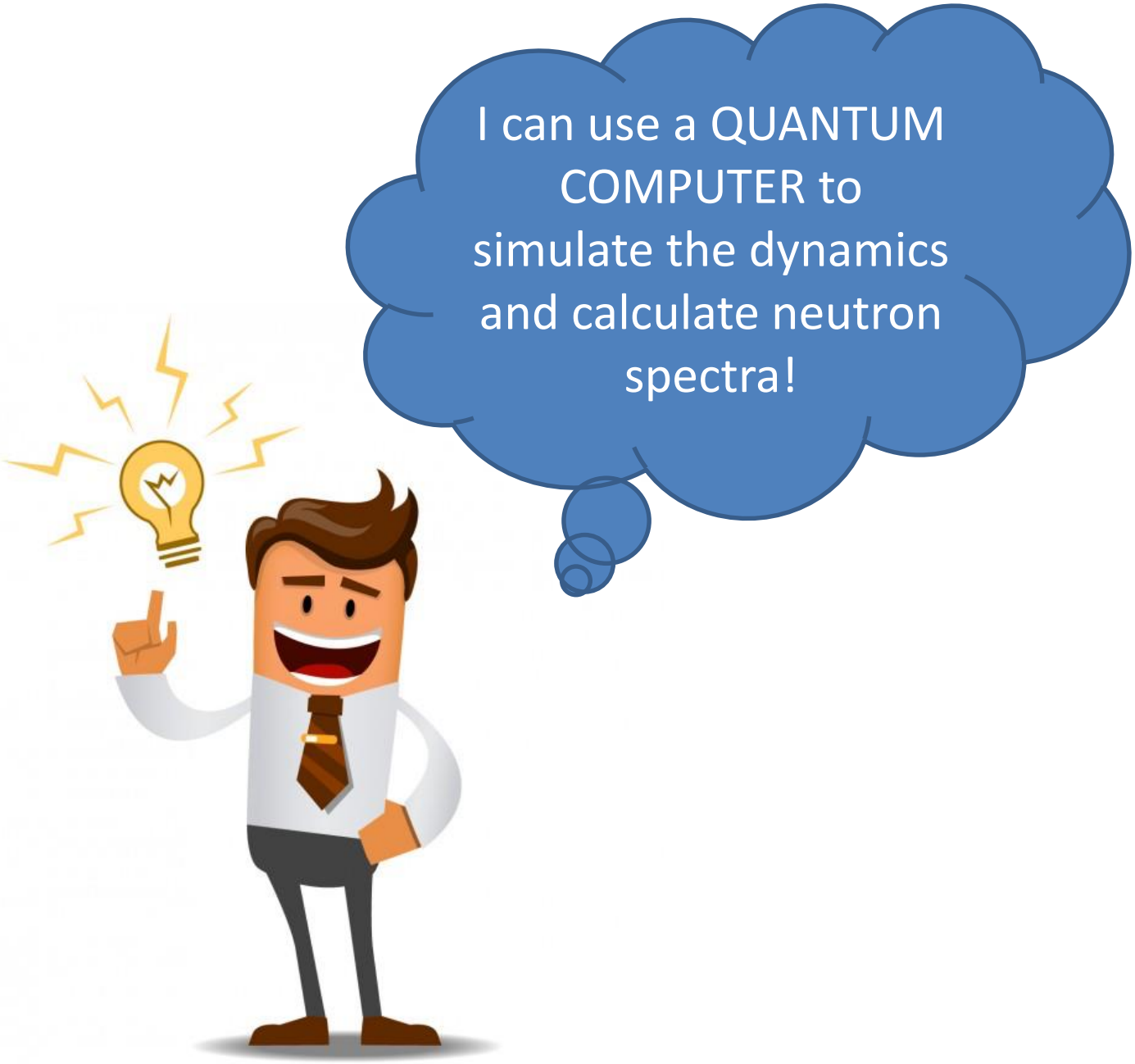


Angew. Chem. Int. Ed. **52**, 9932 (2013)

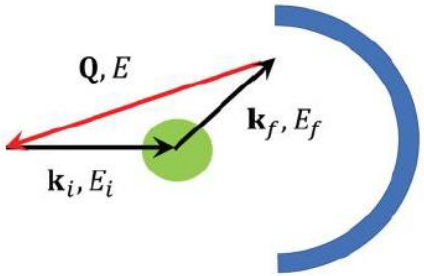
$_{72}Fe_{30}$



Angew. Chem. Int. Ed. **38**, 3238 (1999)
Europhys. Lett. **56**, 863 (2001)


I can use a QUANTUM COMPUTER to simulate the dynamics and calculate neutron spectra!

Magnetic neutron cross-section



$$S(\mathbf{Q},\omega) \propto \sum_{ij}\sum_{\alpha\beta}\sum_{p} \underbrace{F_i(Q)F_j(Q)}\left(\delta_{\alpha\beta} - \frac{Q_\alpha Q_\beta}{Q^2}\right)\langle 0|s_i^\alpha|p\rangle\left\langle p\middle|s_j^\beta\middle|0\right\rangle e^{-i\mathbf{Q}\cdot\mathbf{R}_{ij}}\,\delta\left(\hbar\omega - E_p\right)$$

Atomic Form factors

Positions of magnetic ions

Can be extracted from dynamical correlations functions

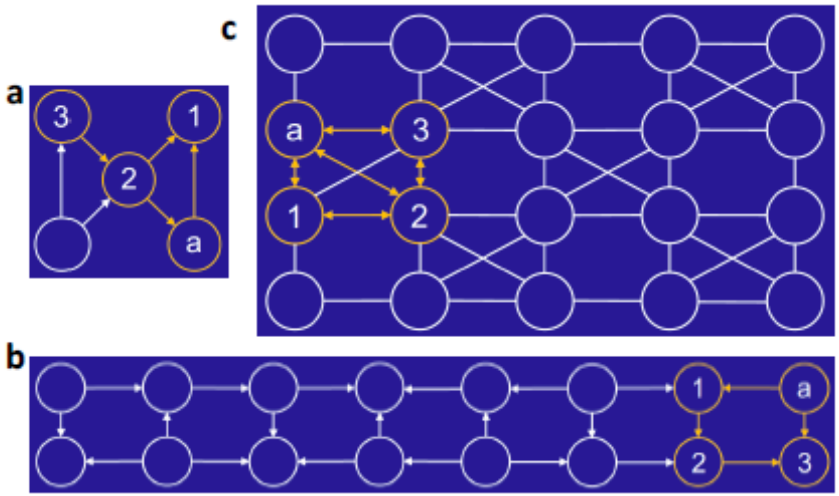
$$C_{ij}^{\alpha\beta}(t) = \left\langle s_i^\alpha(t) s_j^\beta \right\rangle = \sum_p \langle 0|s_i^\alpha|p\rangle\left\langle p\middle|s_j^\beta\middle|0\right\rangle e^{-i\omega_p t} \qquad \omega_p = \frac{E_p - E_0}{\hbar}$$

1. Calculation of $C_{ij}^{\alpha\beta}(t)$ by means of a QC (hard task for a classical device for large number of spins).
2. Obtain $\langle 0|s_i^\alpha|p\rangle\left\langle p\middle|s_j^\beta\middle|0\right\rangle$ and E_p from a QC and easily compute $S(\mathbf{Q},\omega)$ on a classical computer.

Paper submitted

arXiv:1809.07974

We experimentally test this method by computing the INS cross-section for prototypical spin clusters on IBM processors composed of transmon qubits (5- (ibmqx4), 16- (ibmqx5) and 20-qubits (ibmq20)).

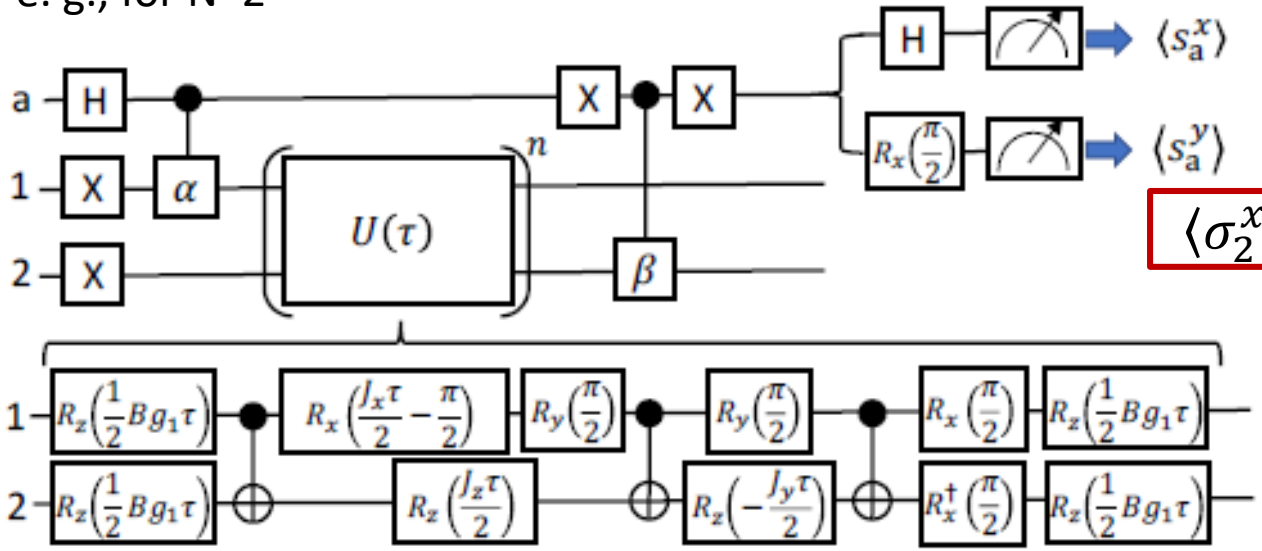


T = 25 mK

$$\mathcal{H} = \sum_{\substack{i=1 \\ \alpha=x,y,z}}^{N-1} J_i^{\alpha} s_i^{\alpha} s_{i+1}^{\alpha} + B \sum_{i=1}^{N} g_i s_i^z$$

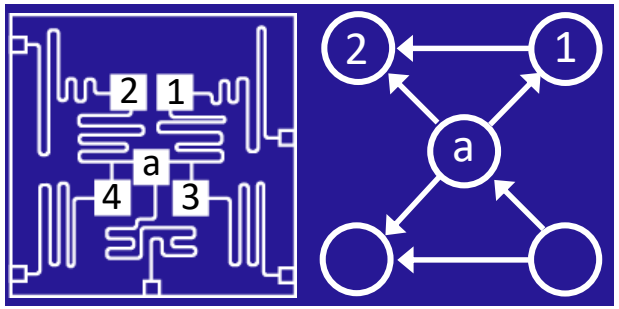
N = 2, 3, 4 (+ ancilla qubit).

e. g., for N=2

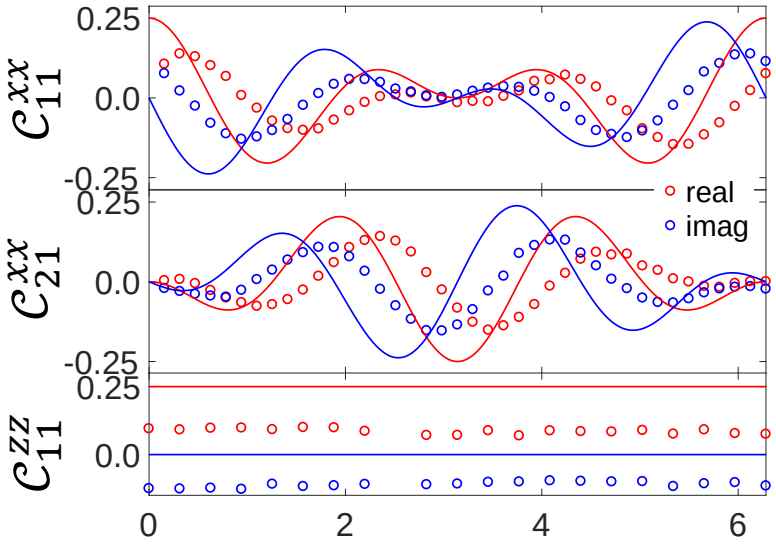


$$\langle \sigma_2^x(t)\sigma_1^x \rangle_{00} = \langle \sigma_a^x \rangle + i\langle \sigma_a^y \rangle$$

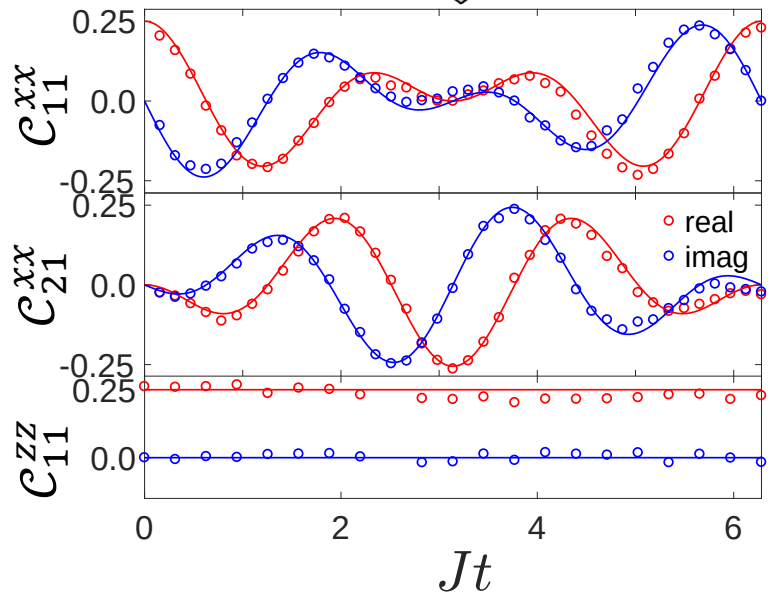
arXiv:1809.07974

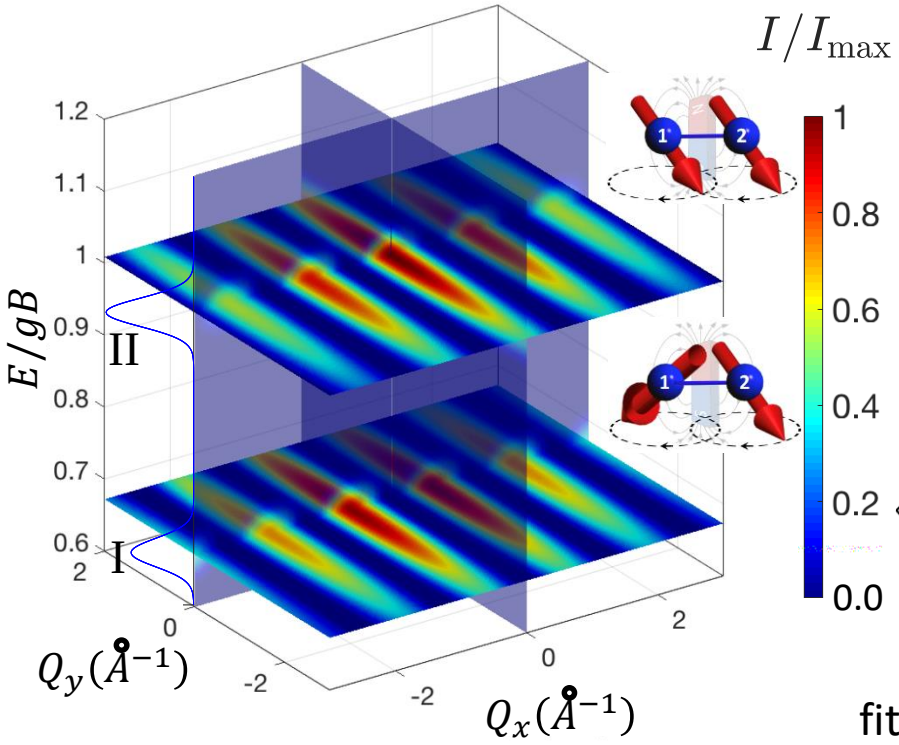


QC



PaS





Cross section

fit

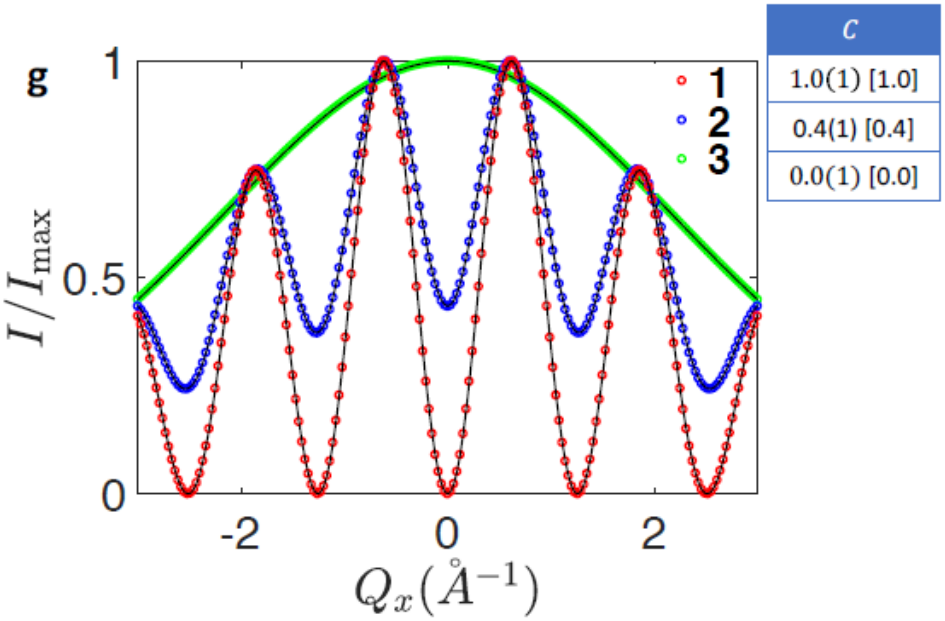
ω_1/J	2.00(2) [2.00]
ω_2/J	3.00(3) [3.00]
$\lvert\langle 0\rvert s_i^x\rvert 1\rangle\rvert^2$	0.125(5) [0.125]
$\langle 0\rvert s_1^x\rvert 1\rangle\langle 1\rvert s_2^x\rvert 0\rangle$	-0.127(5) [-0.125]
$\langle 0\rvert s_1^x\rvert 2\rangle\langle 2\rvert s_2^x\rvert 0\rangle$	0.127(5) [0.125]

Very good agreement with exact calculation!

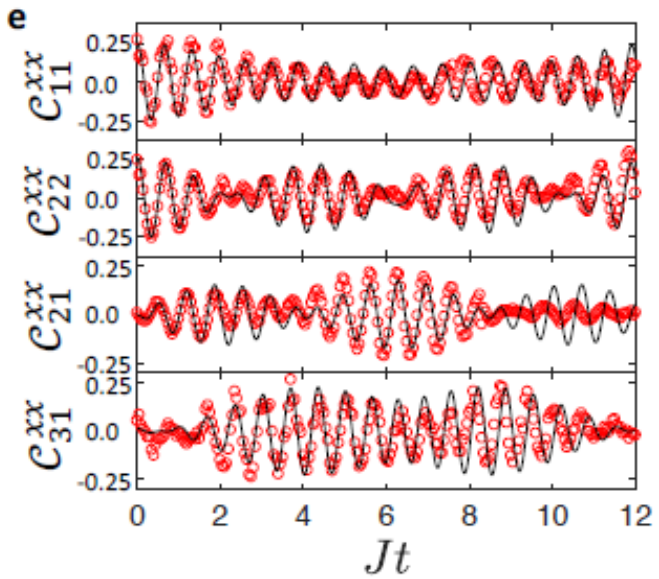
arXiv:1809.07974

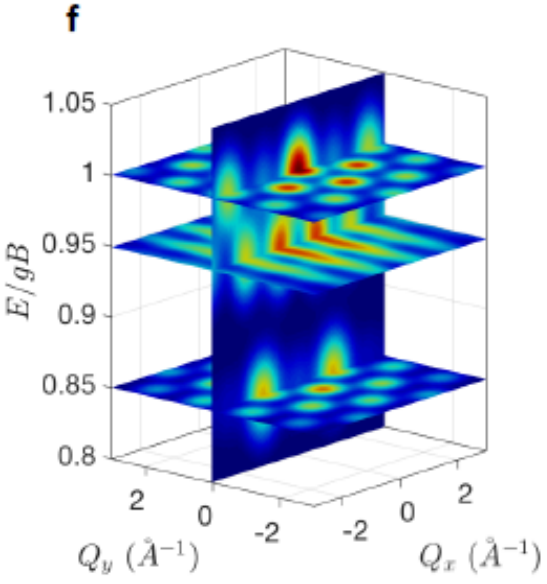
We computed the cross-section of spin dimers characterized by different degrees of entanglement: **1** Heisenberg model, **2** Heisenberg model with inequivalent ions, **3** Ising model.

By focusing on the Q_x-dependence of a single transition: amplitudes of the oscillations fingerprint the degree of entanglement (**Nature Comm. 8, 14543 (2017)**).



For a spin trimer:





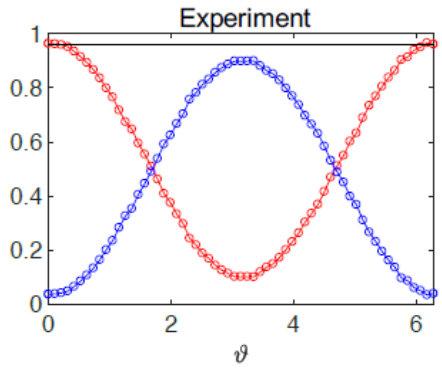
Paper submitted

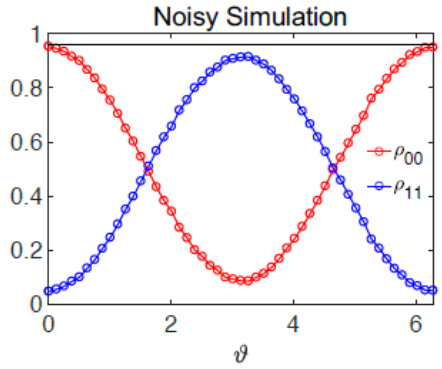
arXiv:1809.07974

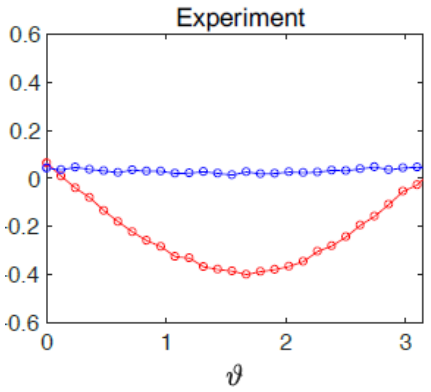
Error assessment and scalability

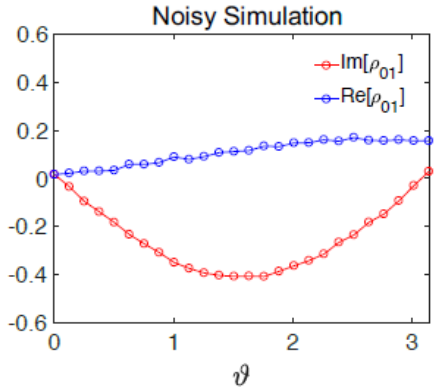
We have studied the various errors and their propagation by comparing targeted experiments on the real hardware to numerical noisy simulations including all main errors: systematic-coherent, measurement and incoherent errors (including relaxation and dephasing).

1) elementary gates: $R_x(\vartheta)$ gate

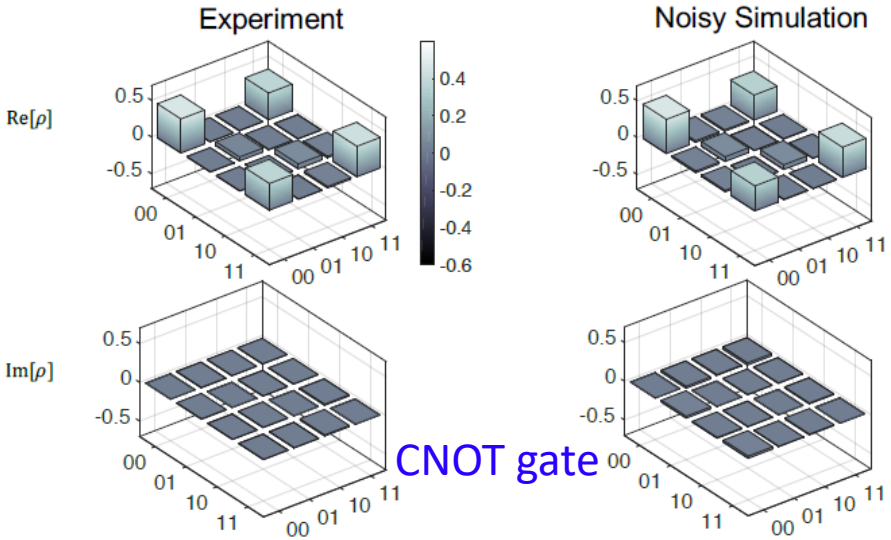






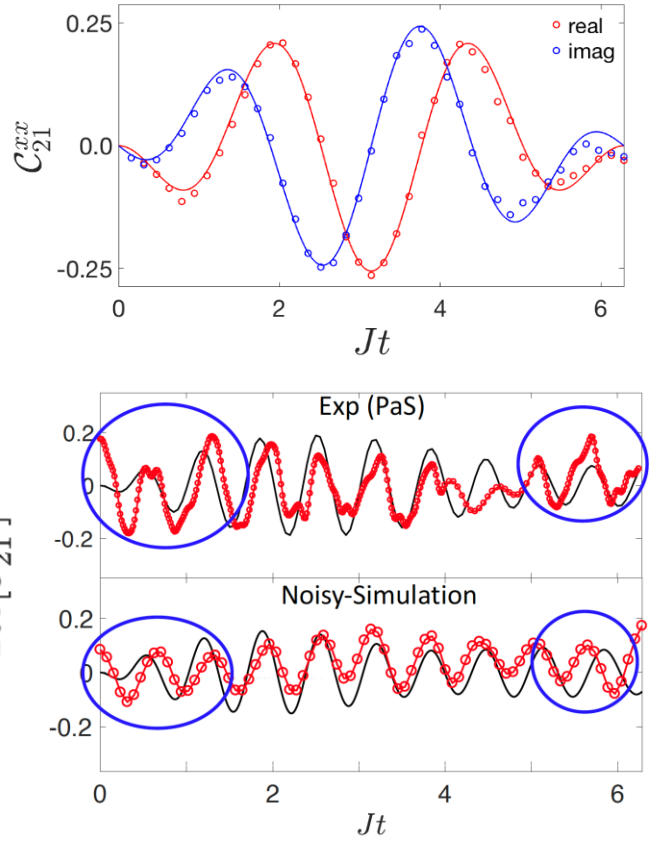


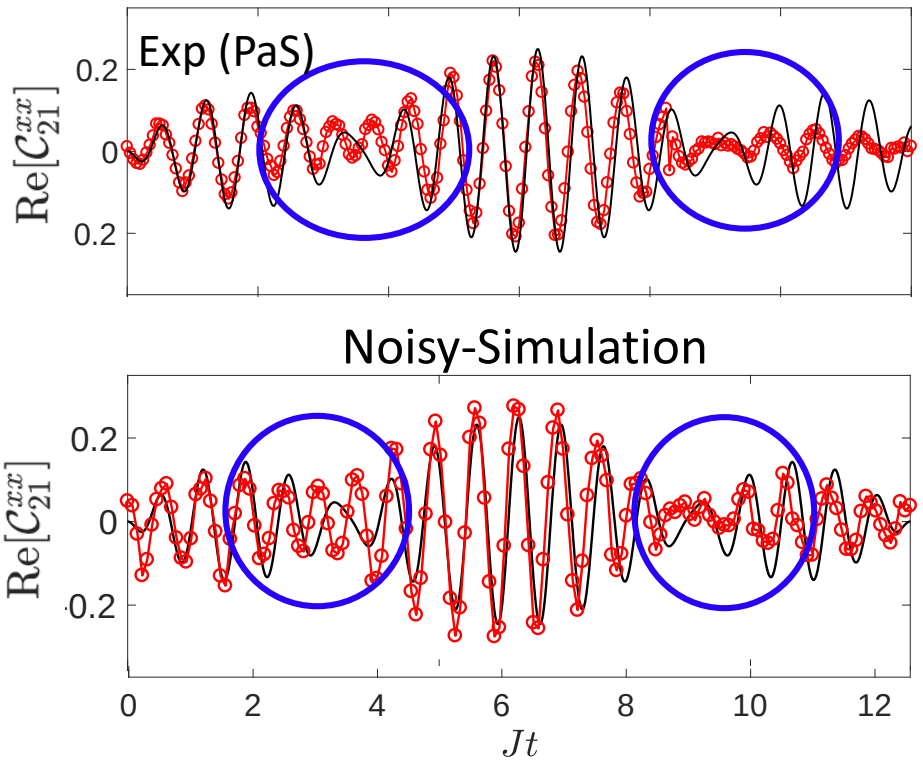
We have quantified all errors and identified SCEs as the leading ones



CNOT gate

To test our error model, we compare the numerical simulation of dynamical correlation functions including errors to experimental results on 3, 4 and 5 qubits (e.g., involving a sequence of 105 noisy gates for N=4).





Different classes of errors can be distinguished:

MOSTLY CORRECTED BY OUR METHOD

-Incoherent Errors essentially yield to an overall attenuation

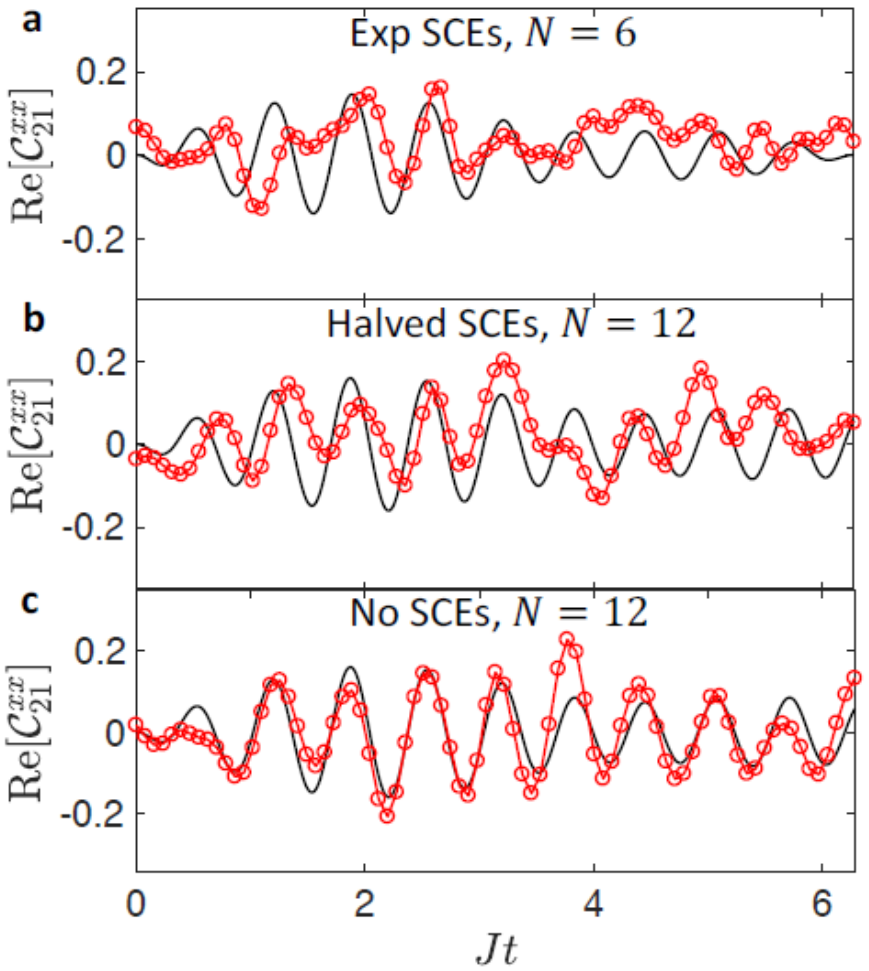
-Concatenation of SCEs can significantly alter the dynamics

Paper submitted

Scalability and near-term perspectives

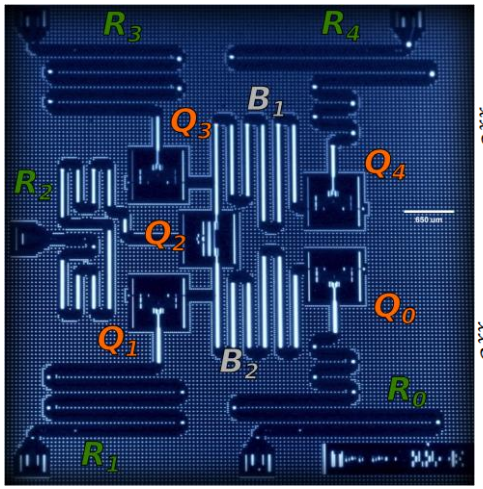
We can now quantitatively investigate the scalability of the method, by including a realistic propagation of errors:

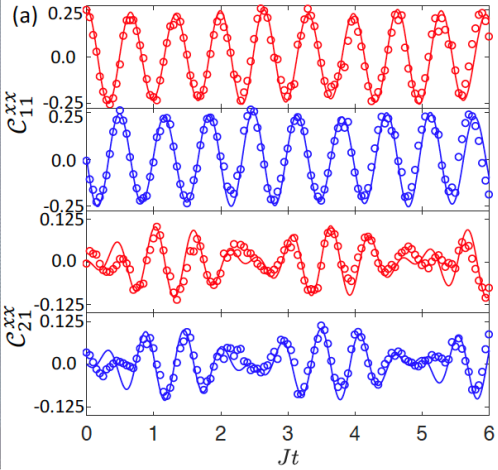
- With current errors the maximum N enabling a reliable computation is ~ 6
- Even a simple halving of SCEs (keeping fixed IEs) would enable a good simulation with N = 12
- by removing the main SCEs and keeping IEs (including T_1, T_2), the simulation for N = 12 is very good



SCEs are currently the main limiting factor and mitigating them is the key to scale to an interesting number of qubits.

Conclusions





- **Quantum simulation** of spin models of interest for physicists and chemists.

- By performing experiments on ibmqx4, ibmqx5, and ibmq20 chips, we show that state-of-the-art (non error-corrected) quantum computers can be used to efficiently calculate the neutron cross-section of finite-size spin systems.

This approach can be extended with forthcoming technological progresses to a number of spins that would make a quantum hardware much faster and efficient than a classical device for the practical interpretation of many experimental data.