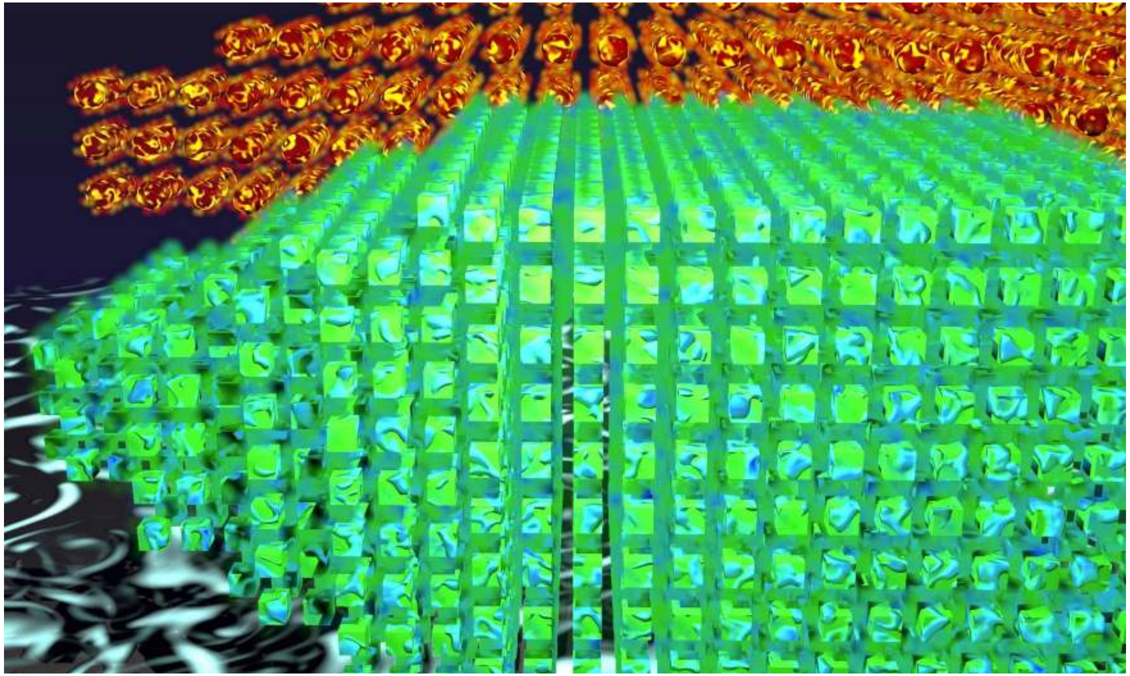
Emulating noisy quantum algorithms with tensor-networks

Jose Lado

Department of Applied Physics, Aalto University, Finland



International symposium on Quantum computing for quantum chemistry and quantum materials science

December 8th 2023, VTT, Finland

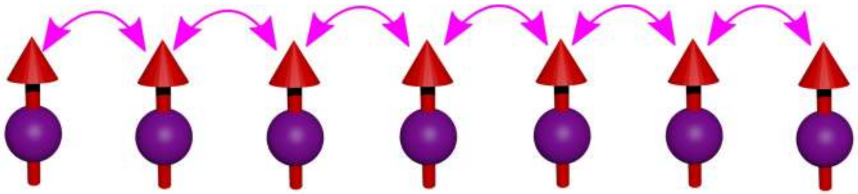
The computational challenge of quantum many-body systems

The problem of dimensionality

In a many-body problem, the size of our vectors grows as

2^L where L is the number of sites

$$\mathcal{H} = \sum_{\langle ij \rangle} J \vec{S}_i \cdot \vec{S}_j$$



For a single-particle problem, we can reach up to 10^8 sites in a laptop

For a many-problem, we cannot even store states for systems bigger than $L = 30$ sites

$$2^{30} \sim 10^9$$

The quantum many-body problem

Let us go back to a simple many-body problem

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

A typical wavefunction is written as

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

We need to determine in total 2^L coefficients

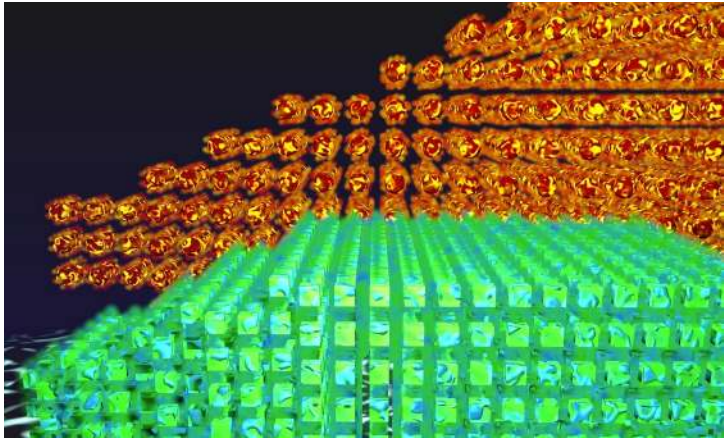
Is there an efficient way of storing so many coefficients?

The fundamental idea of tensor-networks

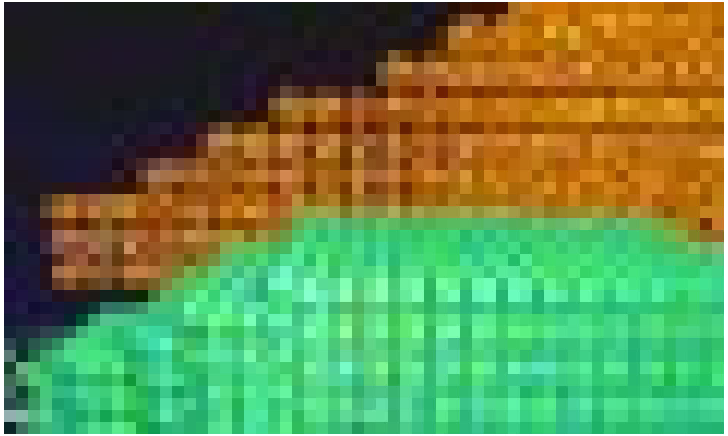
A many-body wavefunction is a very high dimensional object

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

Tensor-networks allow “compressing” all that information in a very efficient way



“True wavefunction”



“Tensor-network wavefunction”

The matrix-product state ansatz

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

Let us imagine to propose a parametrization in this form

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

dimension 2^L

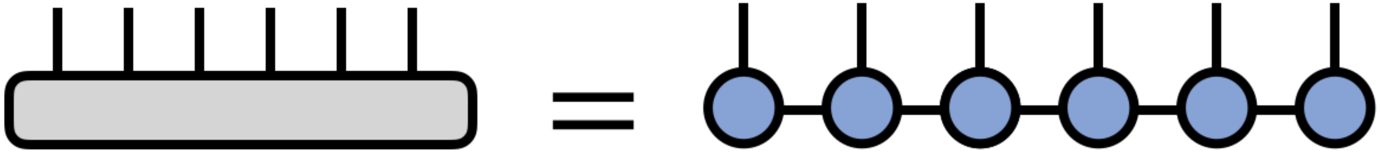
dimension $\sim Lm^2$

(m dimension of the matrix)

State compression with tensor-networks

Given a many-body wavefunction, we can parametrice the components as

$$|\Psi\rangle = \sum_{\{s\}} \mathrm{Tr}\left[M_1^{(s_1)} M_2^{(s_2)} \cdots M_N^{(s_N)} \right] |s_1 s_2 \ldots s_N\rangle$$



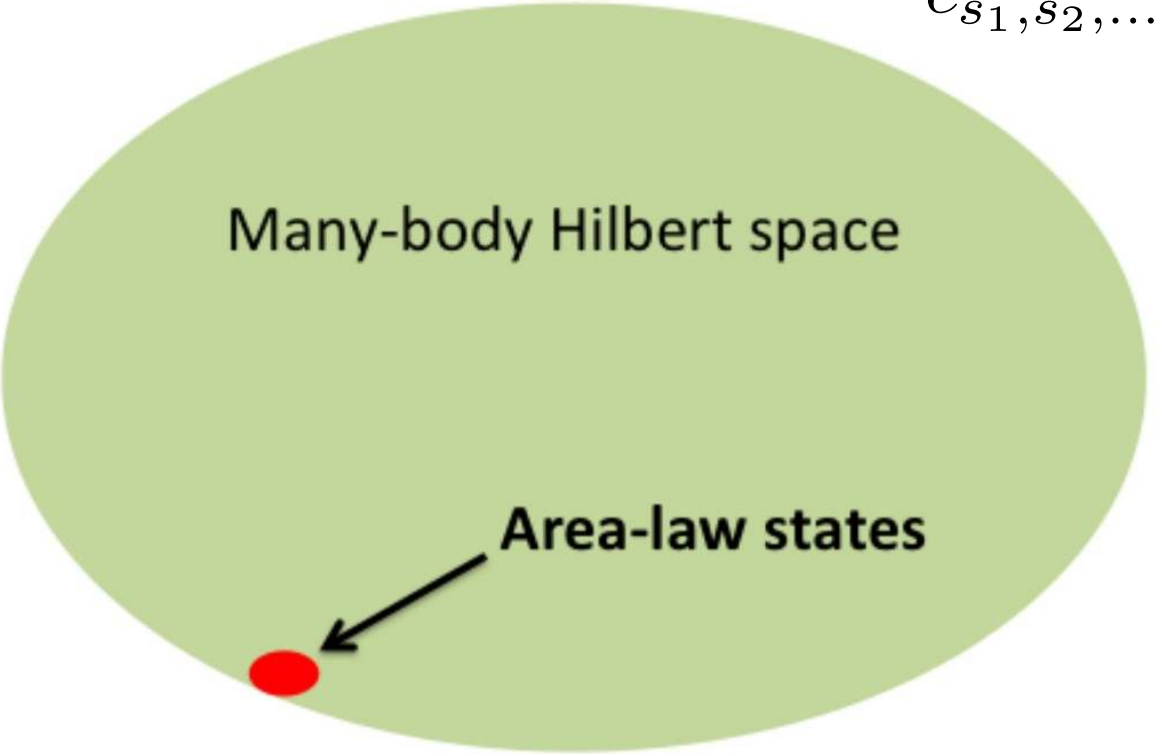
Matrix product state

The previous representation allows drastically reducing the memory required to store a state

Annals of Physics 326, 96 (2011)

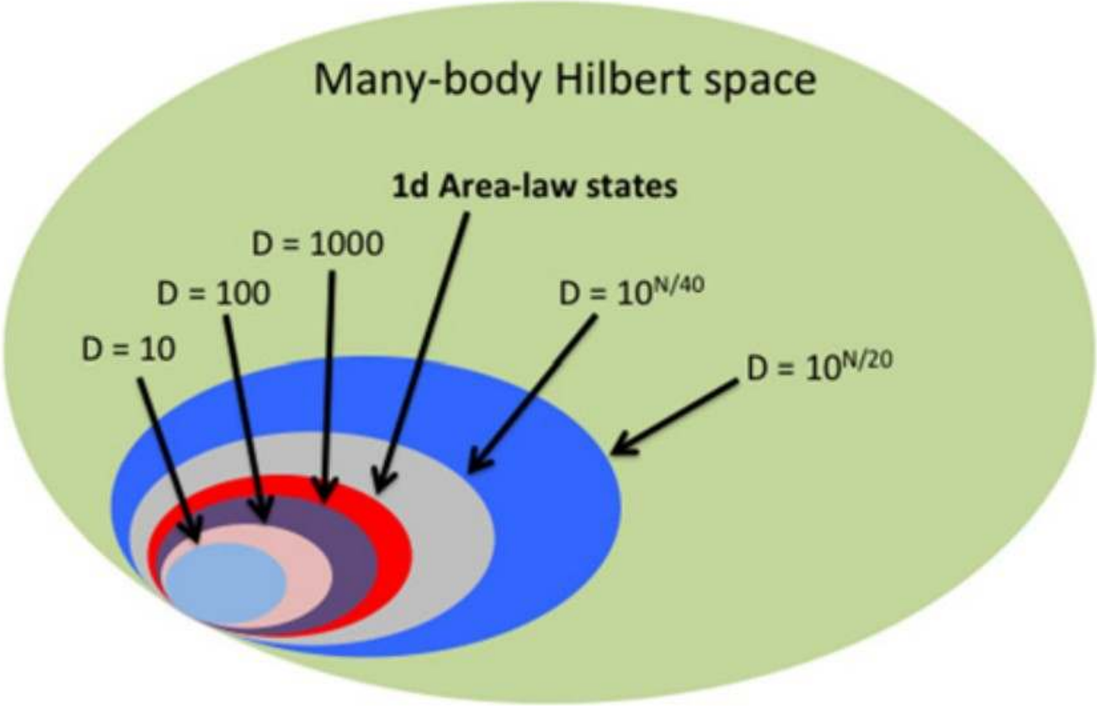
Matrix product states as a parametrization of area law states

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



A controlled way of parametrizing the Hilbert space

Sketch of the space parametrized with bond dimension D



The matrix-product state ansatz

- This ansatz enforces a maximum amount of entanglement entropy in the state $S \sim \log m$
- One-dimensional problems have ground states that can be captured with this ansatz

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

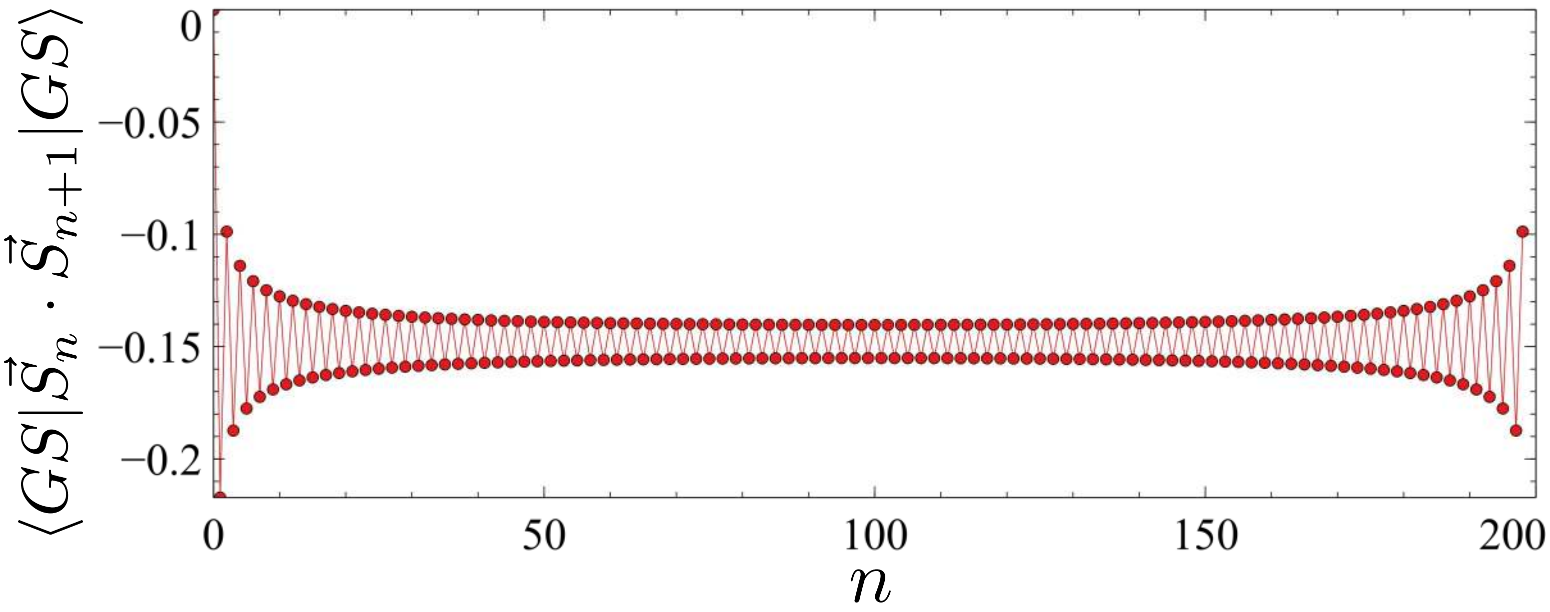
This ansatz can be generalized for time-evolution, excited states, or typical thermal states

The Heisenberg model with tensor-networks

Non-uniform Heisenberg model

$$\mathcal{H} = \sum_n J(n)\vec{S}_n \cdot \vec{S}_{n+1}$$

$$J(n) = J_0 + \delta \cos \Omega n$$

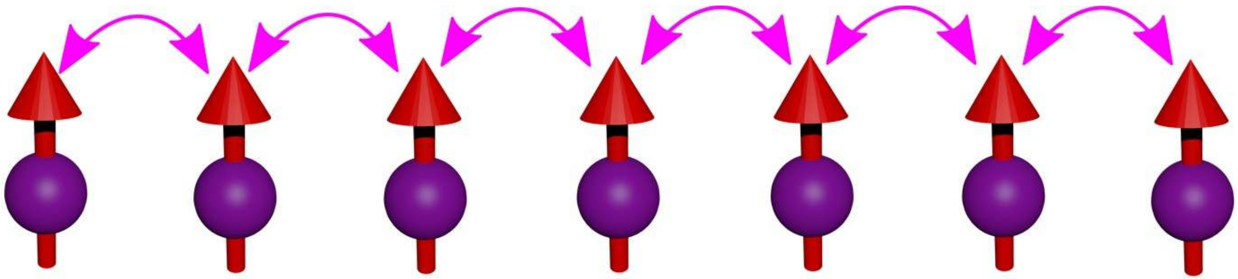


Tensor networks allow solving a 200 many-body spin model in a few seconds in a laptop

Many-body dynamical correlators

One dimensional Heisenberg Hamiltonian

$$\mathcal{H} = \sum_{\langle ij \rangle} J \vec{S}_i \cdot \vec{S}_j$$

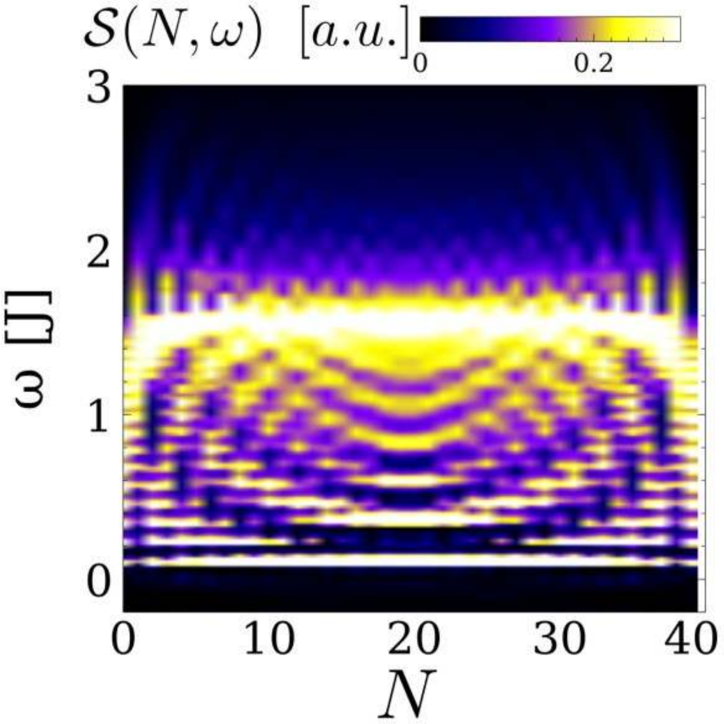


Tensor networks allow computing dynamical correlators

$$\mathcal{S}(N,\omega) = \langle GS | S^z_N \delta(\omega - \mathcal{H} + E_0) S^z_N | GS \rangle$$

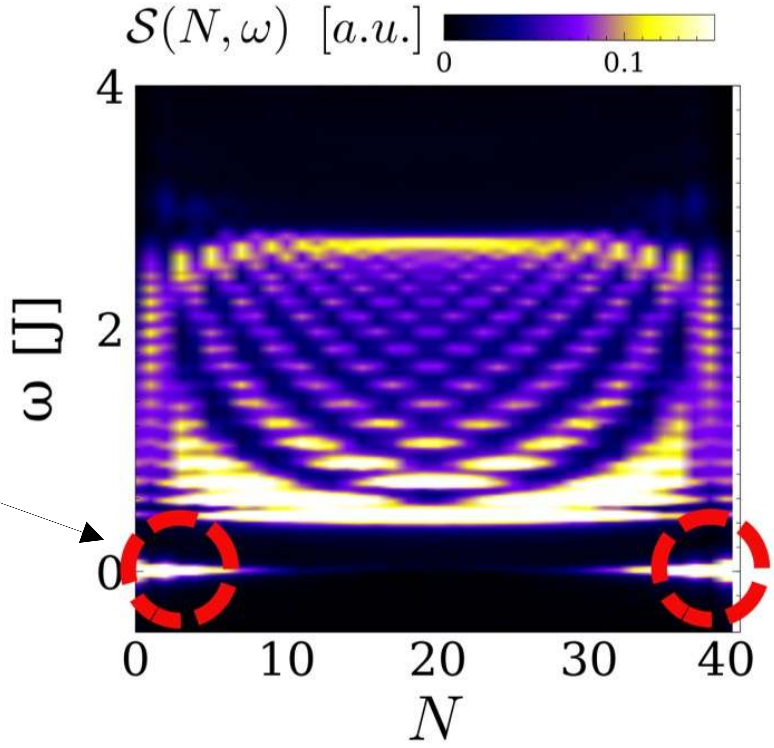
Dynamical structure factor of a Heisenberg model

S=1/2 chain



S=1 chain

Edge modes



Open-source software for tensor-network many-body algorithms

dmrgpy

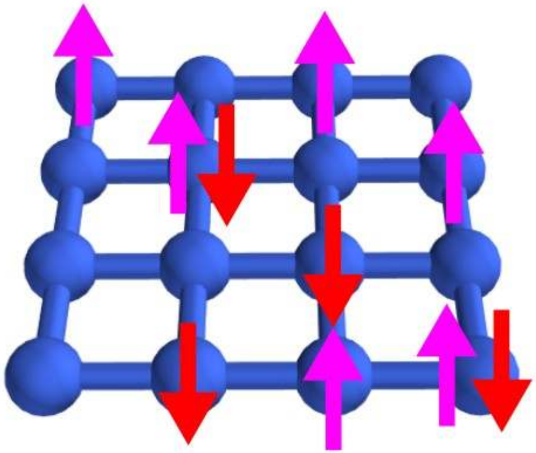
```
from dmrgpy import spinchain
spins = ["S=1" for i in range(40)] # S=1 chain
sc = spinchain.Spin_Chain(spins) # create spin chain object
h = 0 # initialize Hamiltonian
for i in range(len(spins)-1):
  h = h + sc.Sx[i]*sc.Sx[i+1]
  h = h + sc.Sy[i]*sc.Sy[i+1]
  h = h + sc.Sz[i]*sc.Sz[i+1]
sc.set_hamiltonian(h)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

Generic Python library for tensor-network kernel polynomial algorithms for spins, fermions, parafermions, with static and dynamical solvers

https://github.com/joselado/dmrgpy

Some paradigmatic problems solved with matrix product states

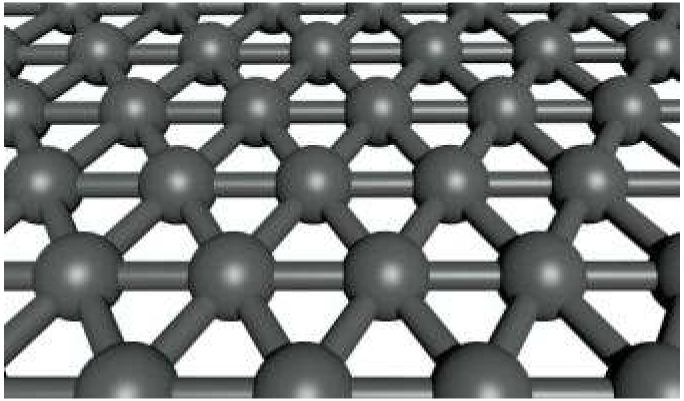
Solving the 2D Hubbard model at finite doping



$$H = \sum_{ij,s} t_{ij} c^\dagger_{is} c_{js} + \sum_i U c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$

Science, 365(6460), 1424-1428 (2019)

Solving the 2D Heisenberg model in frustrated lattices



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

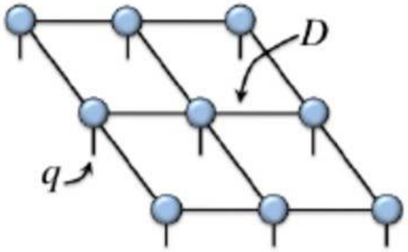
Phys. Rev. Lett. 123, 207203 (2019)

Many-body state compression

Matrix-product states

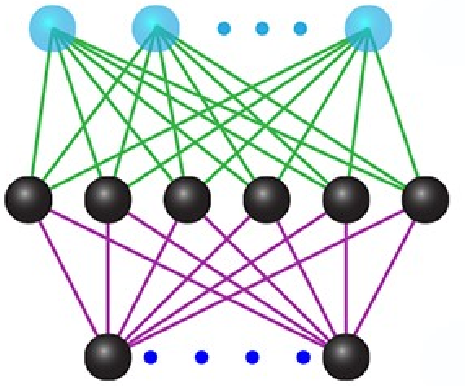
Phys. Rev. Lett. 69, 2863 (1992)

Projected entangled pair-states



Annals of Physics 326, 96 (2011)

Neural-network quantum states



Science 355.6325 (2017): 602-606.

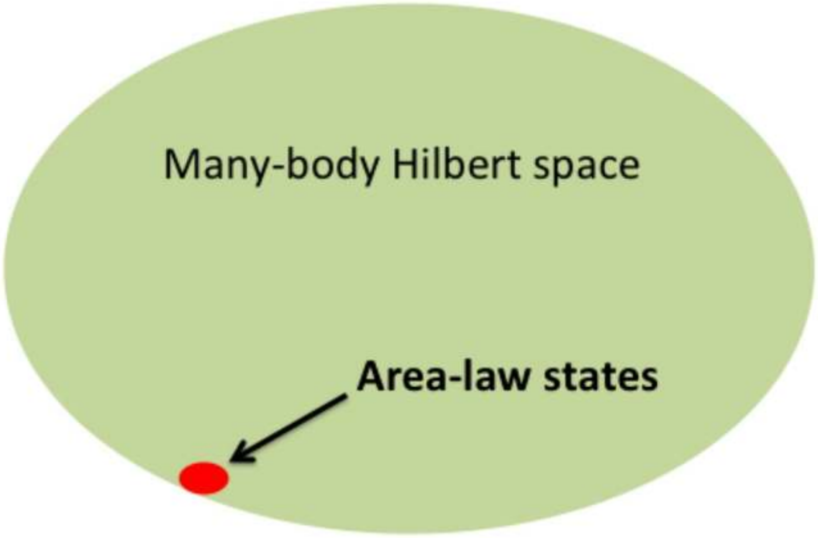
Other compressed many-body states could be potentially used for noisy quantum circuit simulation

Tensor-networks for noisy quantum circuits

How much entanglement do we need

Qubit fidelity limits which states we can create in a quantum circuit

Tensor-network bond dimension limits which states we parametrize



<u>Both constrains put bounds to the entanglement of accessible states</u>

Phys. Rev. X 10, 041038 (2020)

Do we need the whole Hilbert space to successfully run a quantum algorithm?

Could we get meaningful results even if we can only access part of the Hilbert space?

Behind the scenes

Marcel Niedermeier

Marc Nairn

Christian Flindt

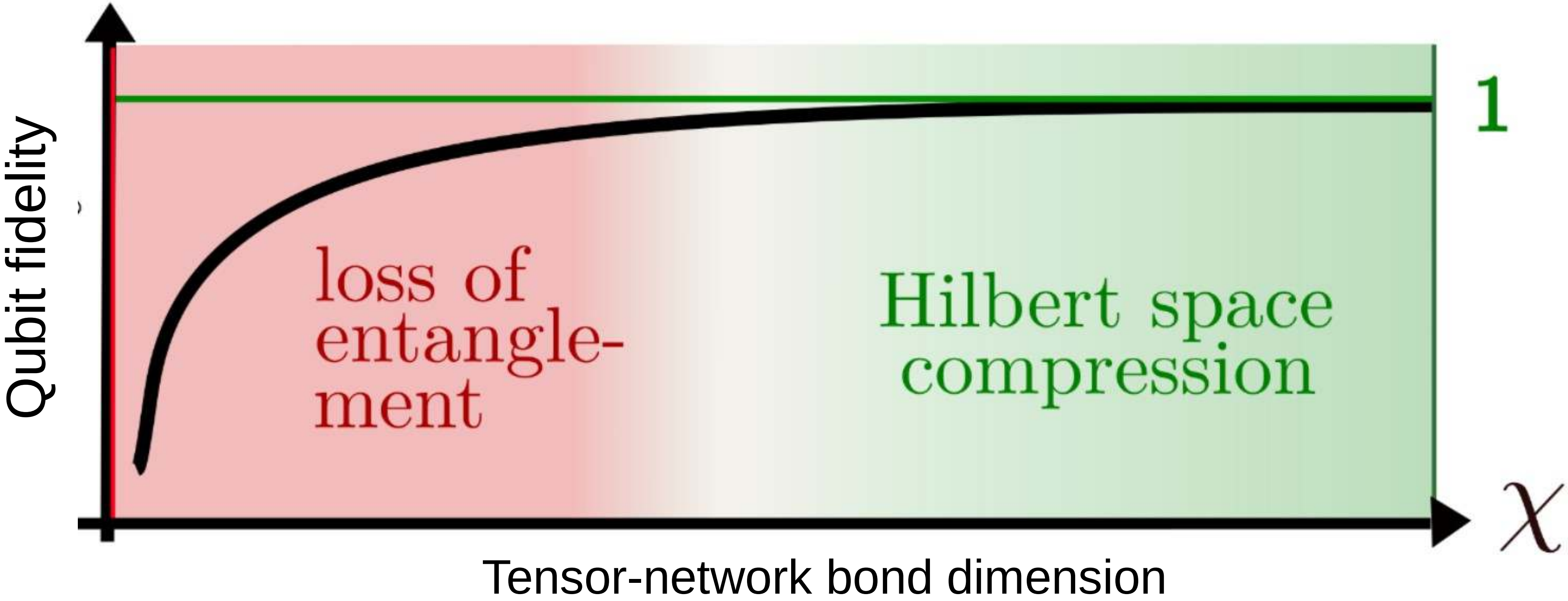
Noisy quantum circuit algorithms with tensor networks

M. Niedermeier, J. L. Lado, C. Flindt, arXiv:2304.01751 (2023)

Computing topological invariants with noisy quantum circuits

M. Niedermeier, M. Nairn, C. Flindt, J. L. Lado, to appear (2024)

What is the relation between a noisy qubit and a tensor network?



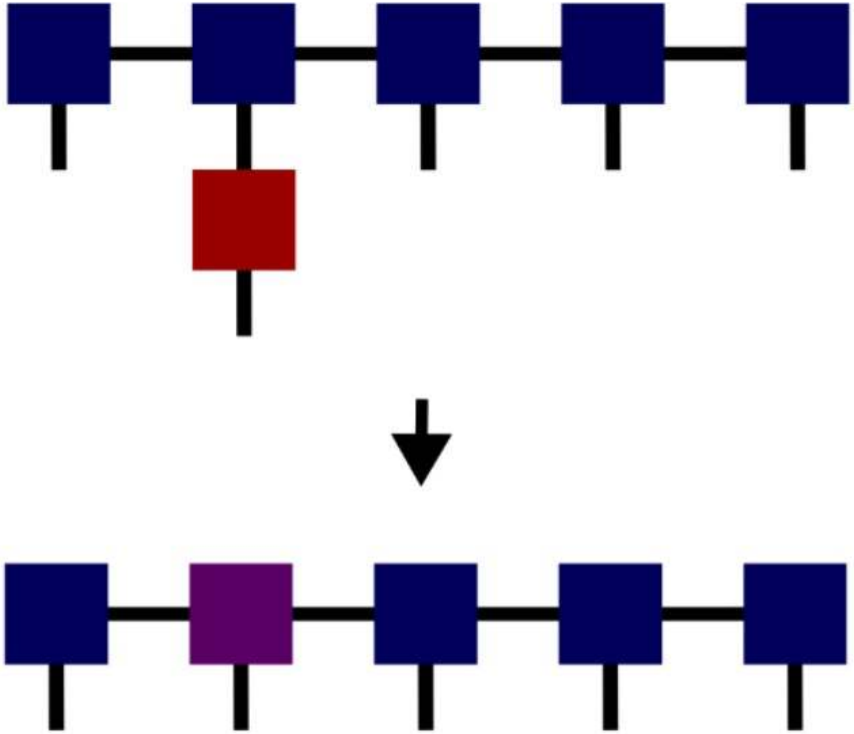
The finite tensor-network bond dimension can be understood as a finite qubit fidelity

Applying a single qubit gate to a tensor network

Original MPS

Single qubit gate

Transform MPS



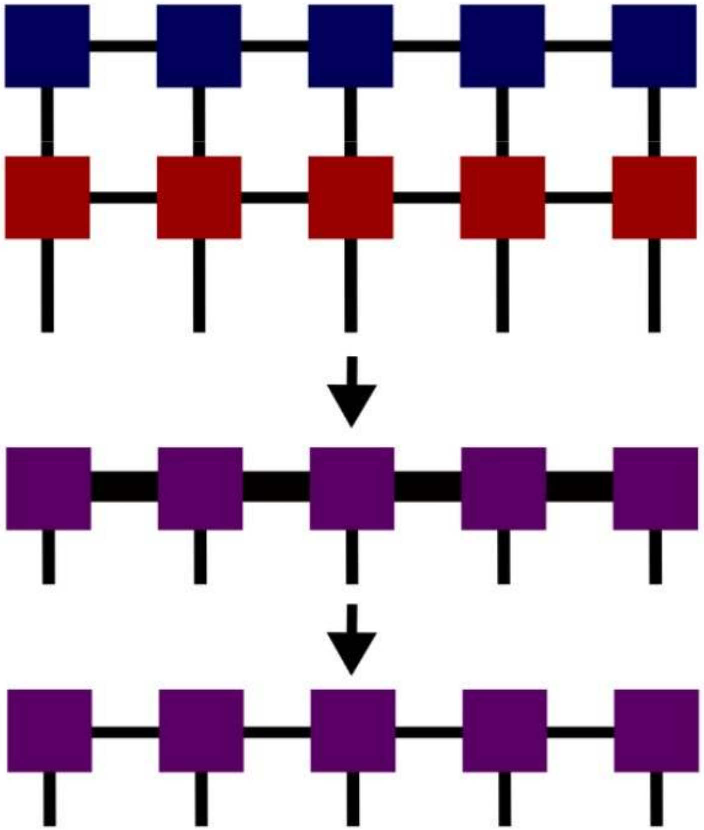
Applying a multi-qubit gate to a tensor network

Original MPS

Multi-qubit gate

Higher dimension updated MPS

Compressed updated MPS

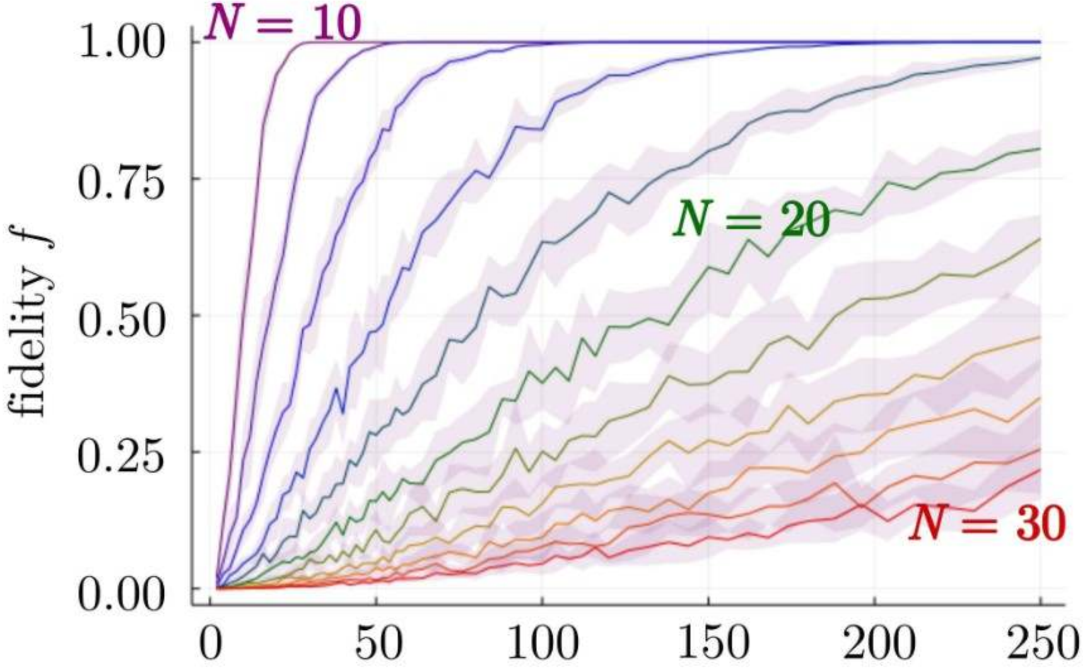


Three quantum algorithms with tensor-network quantum circuits

- ***Quantum Fourier transform:*** quantum analogue of the discrete Fourier transform
- ***Grover's algorithm:*** find elements in a database
- ***Quantum counting algorithm:*** counting the number of solutions for a given search problem

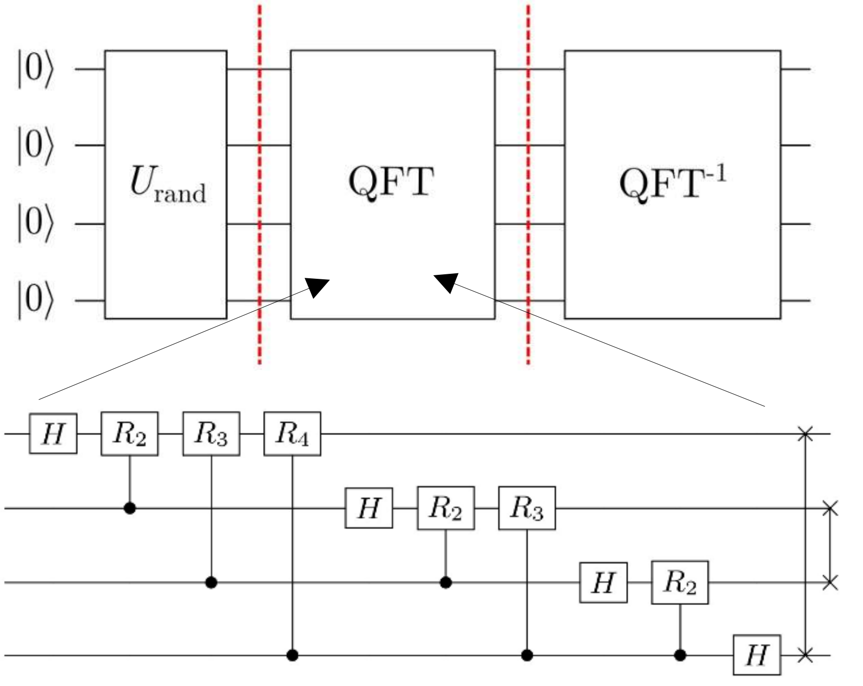
The quantum Fourier transform

N is the number of qubits



Tensor-network bond dimension

Circuit architecture



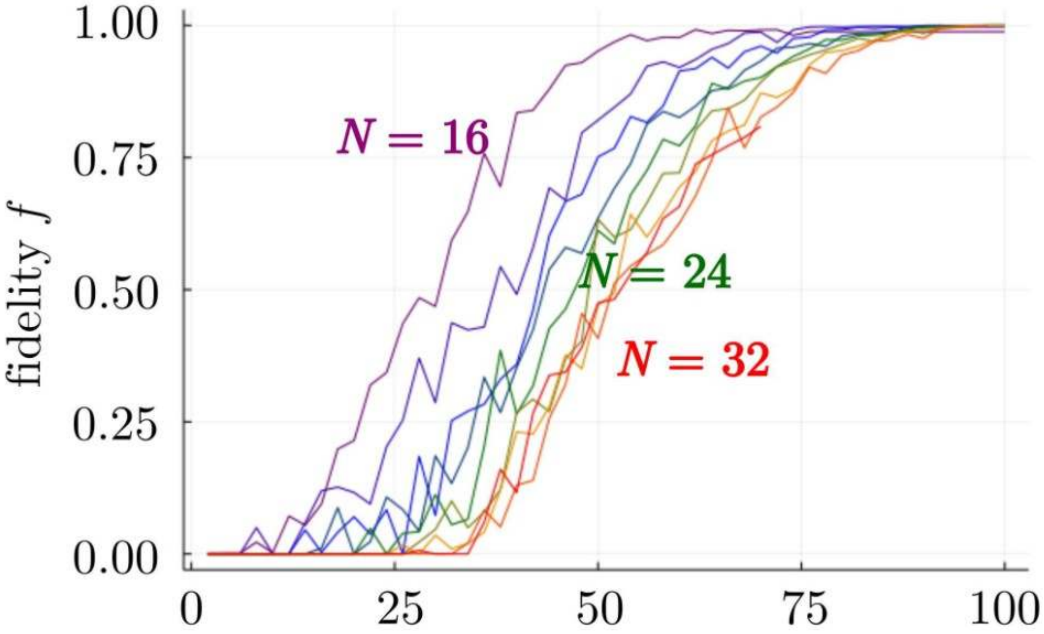
QFT Fidelity

$$f = |\langle \Psi_0' | \Psi_0 \rangle|^2 \qquad |\Psi_0'\rangle = \text{QFT}^{-1}\text{QFT}\,|\Psi_0\rangle$$

arXiv:2304.01751 (2023)

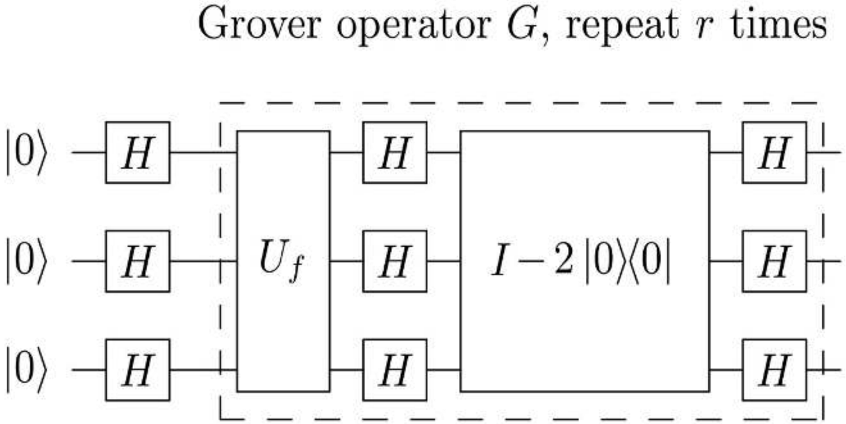
Grover’s search algorithm

N is the number of qubits



Tensor-network bond dimension

Circuit architecture



Grover fidelity (m marked elements)

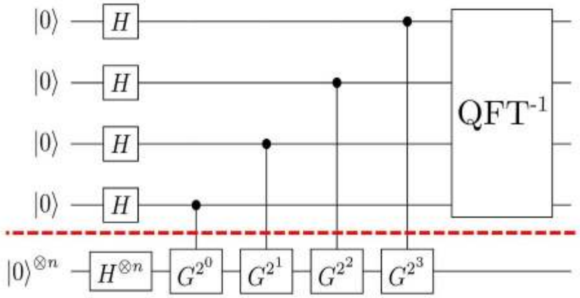
$$f_r = \frac{1}{m}\sum_{i}^{m} |\,\langle \omega_i|\Psi_r\rangle\,|^2$$

arXiv:2304.01751 (2023)

Quantum counting algorithm

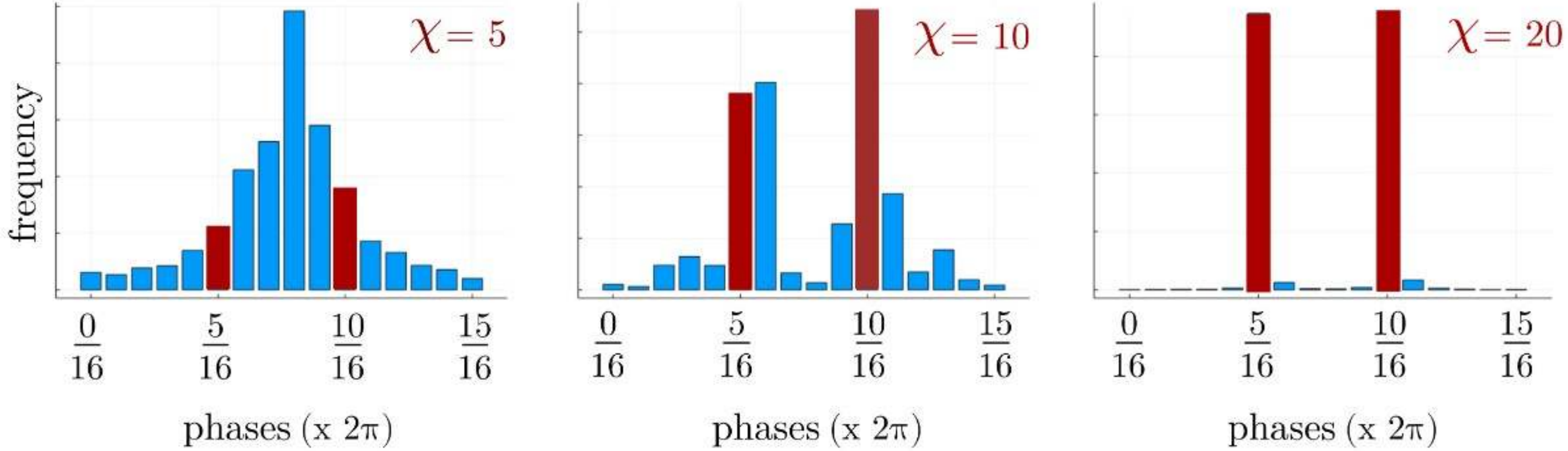
arXiv:2304.01751 (2023)

Circuit architecture



Phases of marked elements (correct in red)

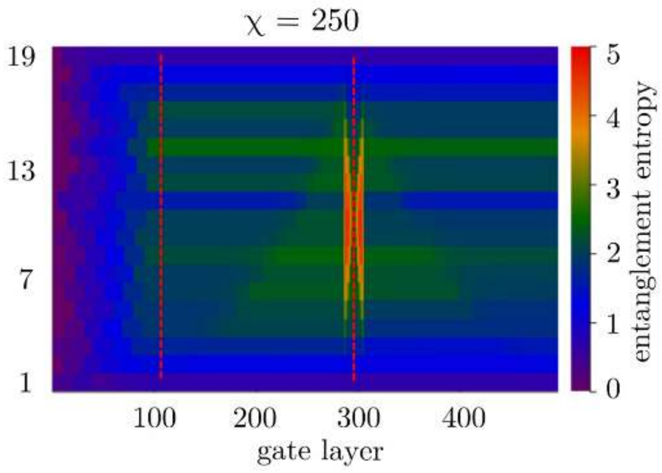
low-quality circuit



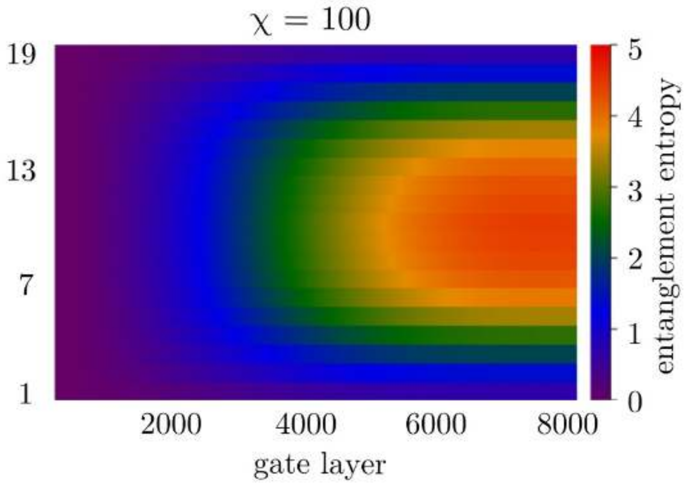
high-quality circuit

Entanglement propagation in the quantum-circuit

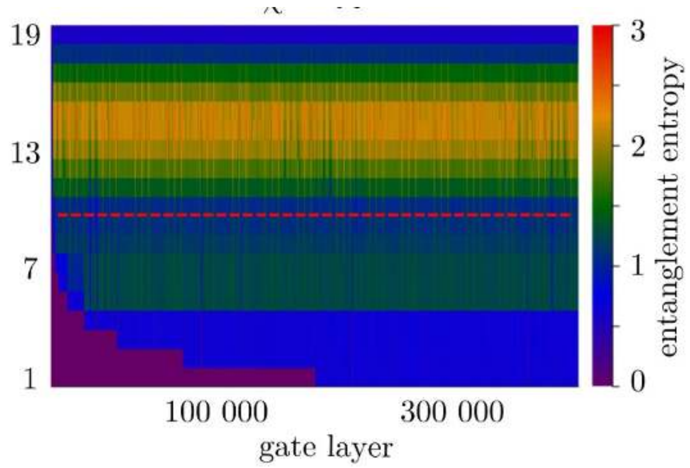
Quantum Fourier transform



Grover's algorithm



Quantum counting algorithm



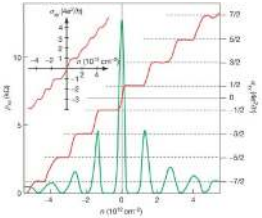
Entanglement builds up in concrete locations and steps of the quantum circuit

arXiv:2304.01751 (2023)

Quantum circuits for topological quantum materials

Topological quantum matter

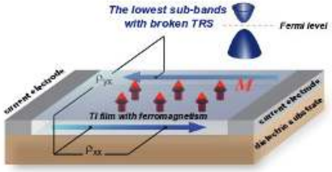
Quantum Hall effect



graphene

Nature 438, 197-200 (2005)

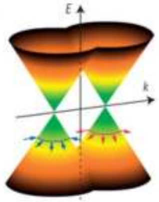
Quantum Anomalous Hall effect



Cr-doped $(Bi,Sb)_2Te_3$

Science 340.6129 (2013): 167-170

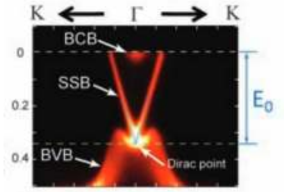
Weyl semimetal



TaAs

Nature Physics 11, 724–727 (2015)

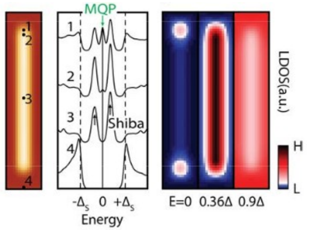
Quantum Spin Hall effect



Bi_2Se_3

Science 325.5937 (2009): 178-181

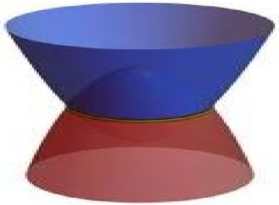
Topological superconductor



Fe@Pb

Science 346.6209 (2014): 602-607

Nodal line semimetals



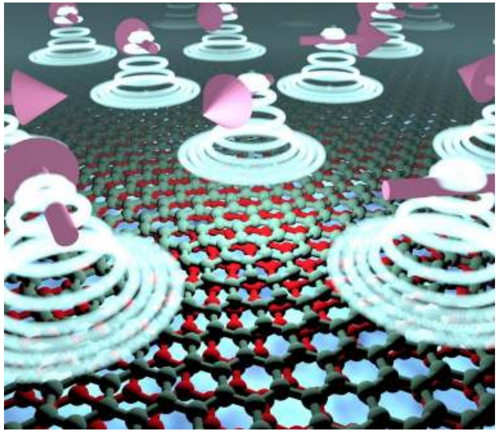
Mg_3Bi_2

Advanced Science 6.4 (2019): 1800897

All these states are described by effective isolated single-particle Hamiltonians

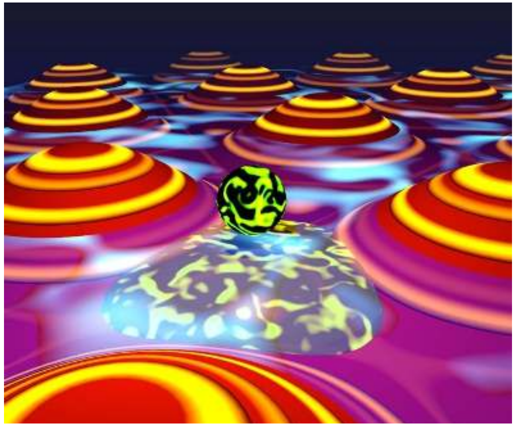
Many-body topological quantum matter

Quantum spin liquids



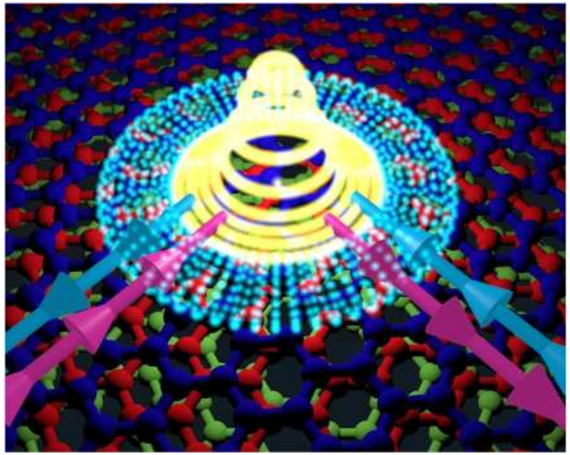
Reports on Progress in Physics 80.1 (2016): 016502.

Fractional Chern insulators



Rev. Mod. Phys. 71, S298 (1999)

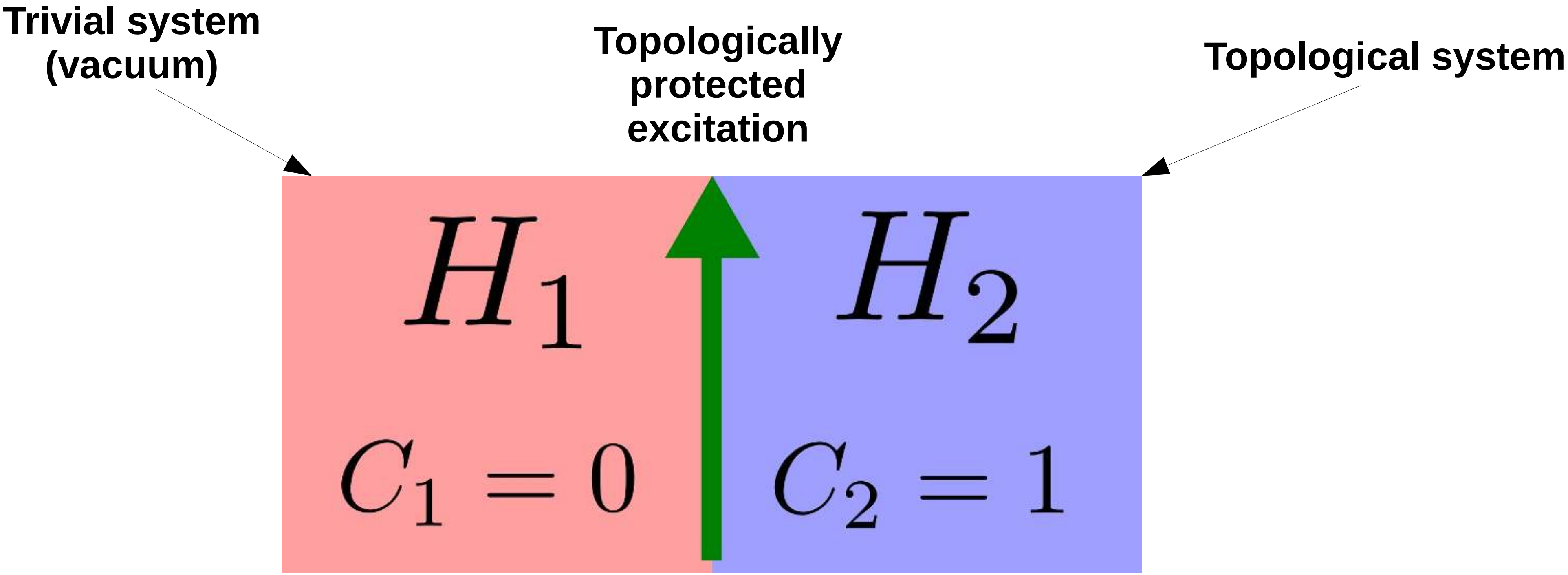
Parafermions



Annual Review of Condensed Matter Physics 7, 119-139 (2016)

Topological many-body quantum matter is an open challenge where quantum algorithms will potentially enable major breakthroughs

The consequence of different topological invariants

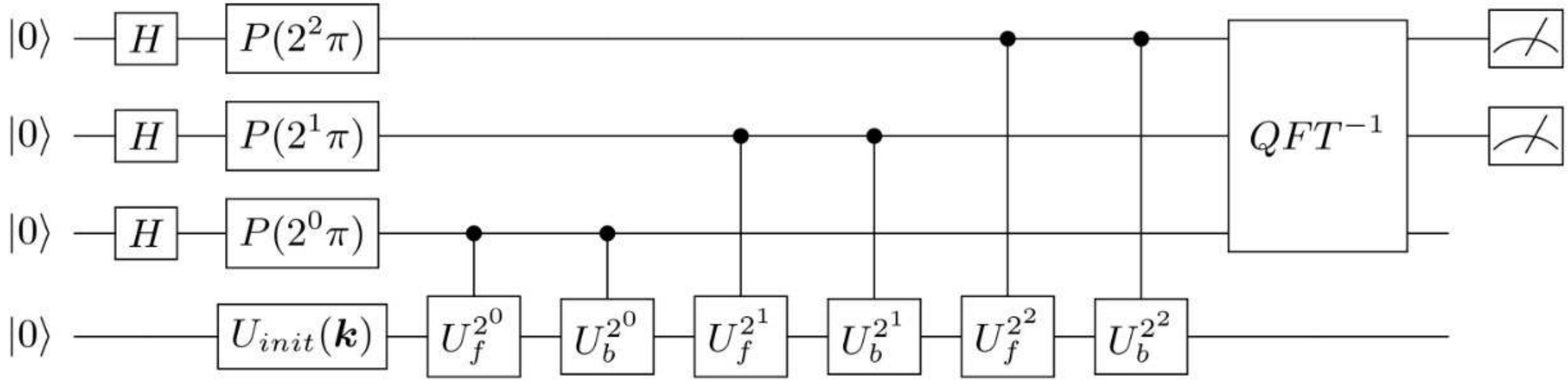


Topological excitations appear between topologically different systems

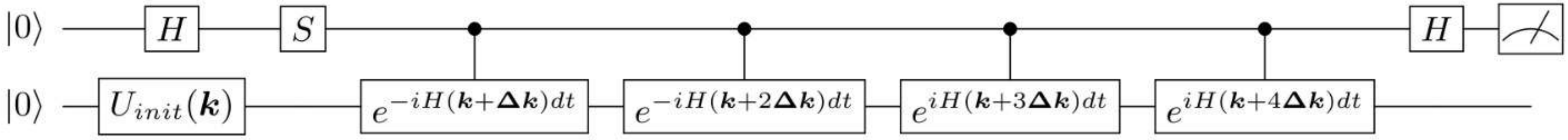
<u>Topological invariants are integers, and thus potentially robust in noisy quantum circuits</u>

Quantum circuits to compute topological invariants

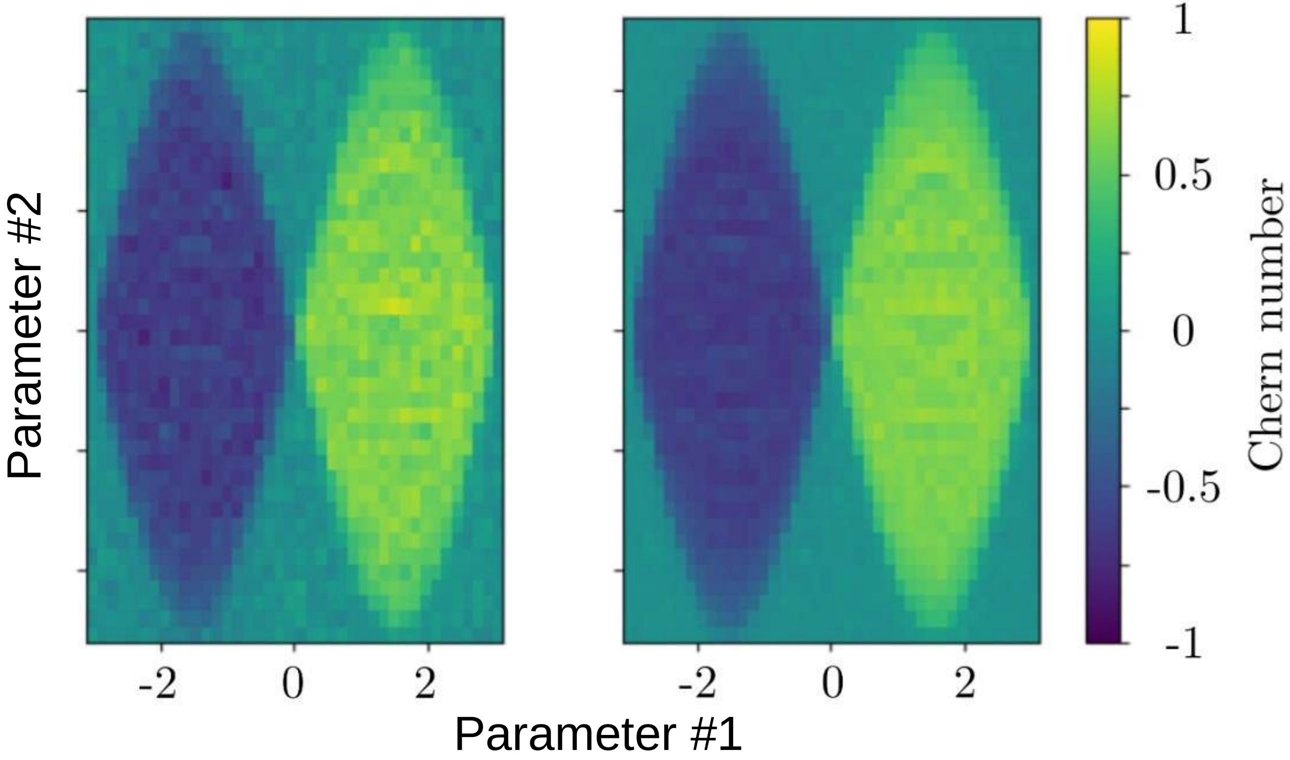
Berry phase (topological invariant for 1D materials)



Chern number (topological invariant for 2D materials)



Topological invariants computed with a quantum circuit

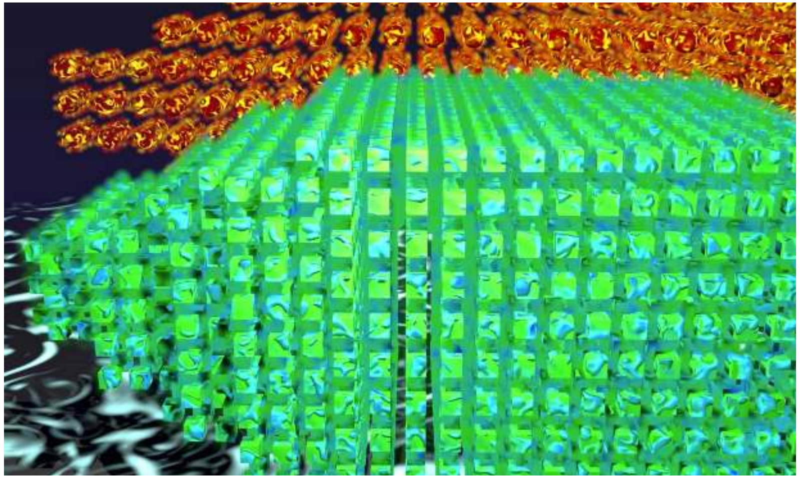


Topological invariants can be extracted even from noisy quantum circuits

M. Niedermeier, M. Nairn, C. Flindt, J. L. Lado, to appear (2024)

Take home

Tensor-networks offer a promising strategy to benchmark how quantum algorithms perform in large noisy quantum circuits



arXiv:2304.01751 (2023)

Funding from

Thank you