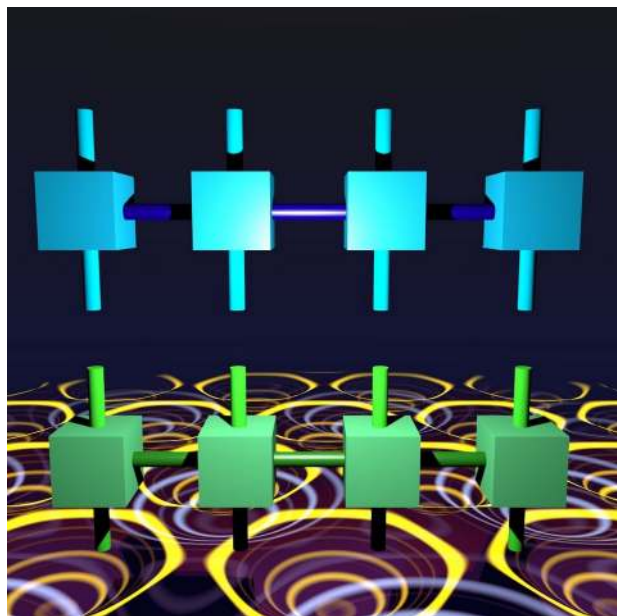


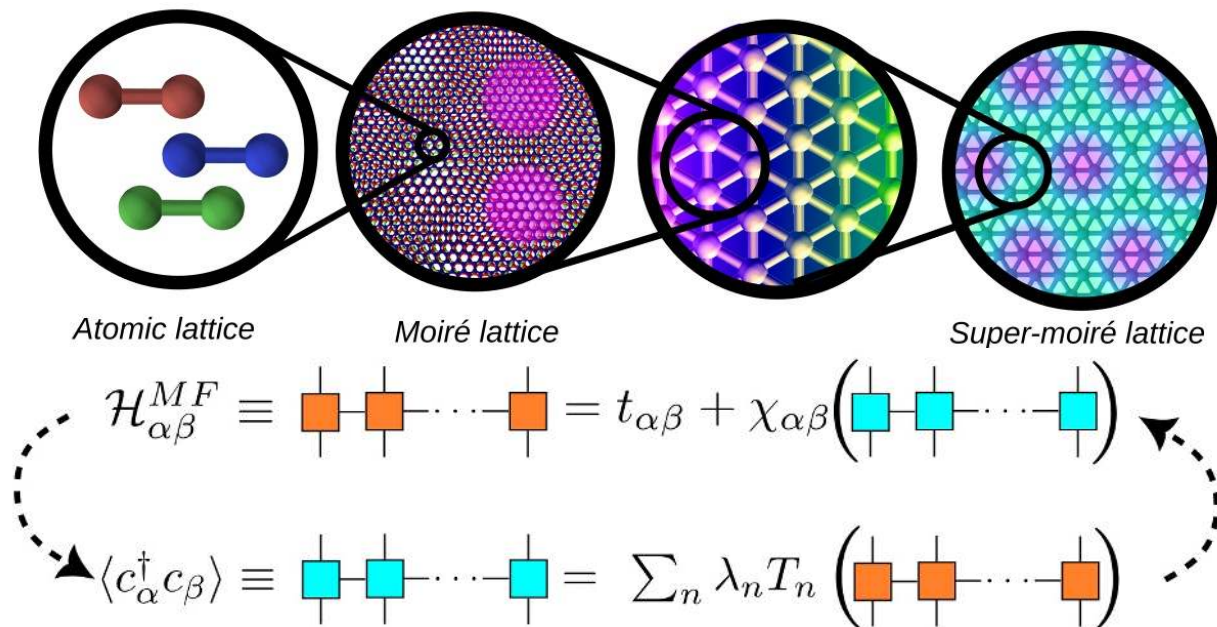
Solving correlated super-moire materials beyond one billion sites with tensor networks

Jose Lado

Department of Applied Physics, Aalto University, Finland



2D Materials 12 (1), 015018 (2025)



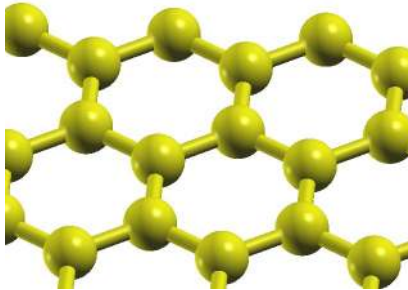
arXiv:2503.04373 (2025)

arXiv:2506.05230 (2025)

The two-dimensional materials world

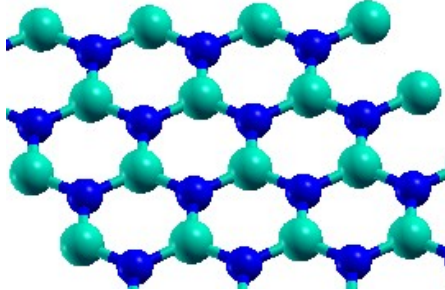
Semimetal

Graphene



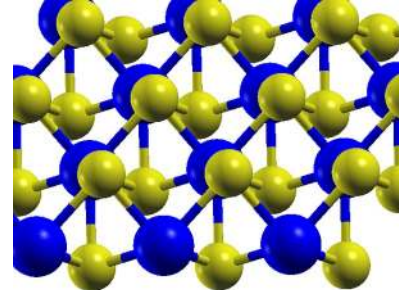
Insulator

BN



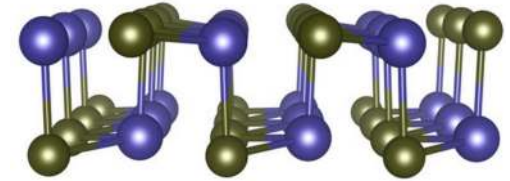
Superconductor

NbSe₂



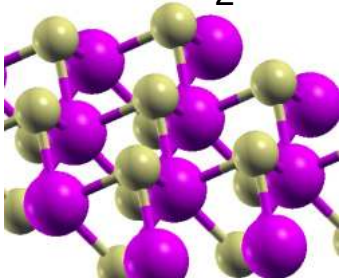
Ferroelectric

SnTe



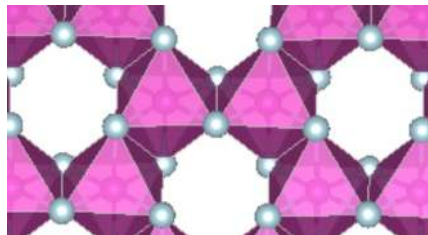
Semiconductor

WS₂



Ferromagnet

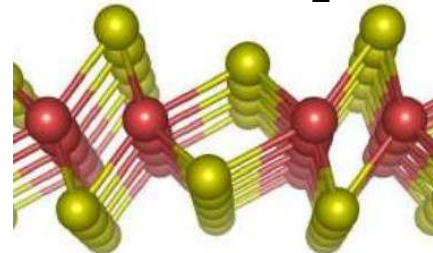
CrI₃



Quantum spin

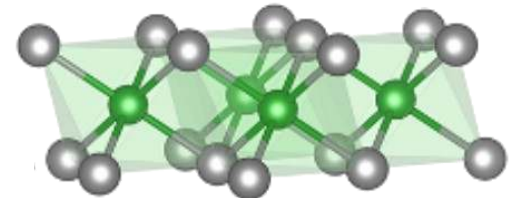
Hall insulator

WTe₂



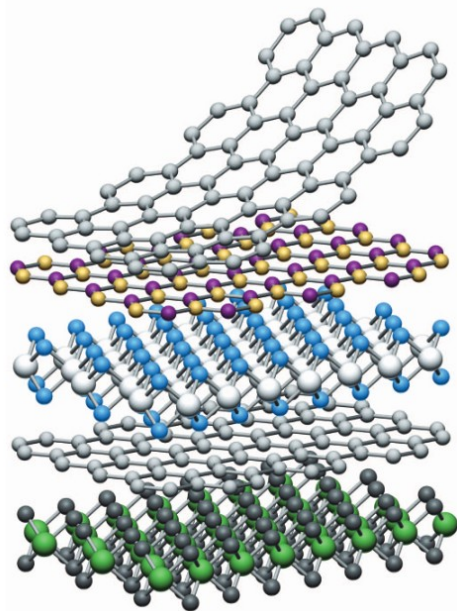
Multiferroic

NiI₂



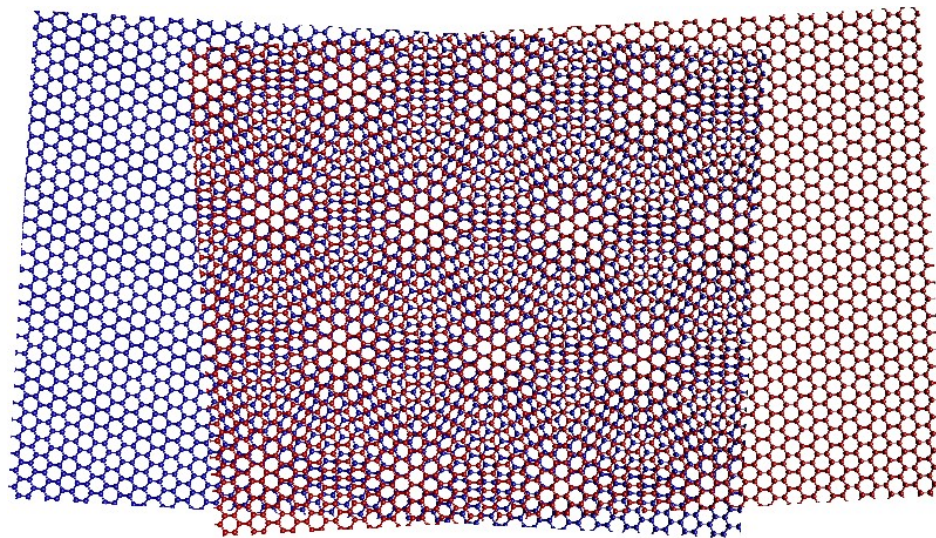
The flexibility of two-dimensional materials

They can be stacked



Nature 499, 419–425 (2013)

They can be rotated

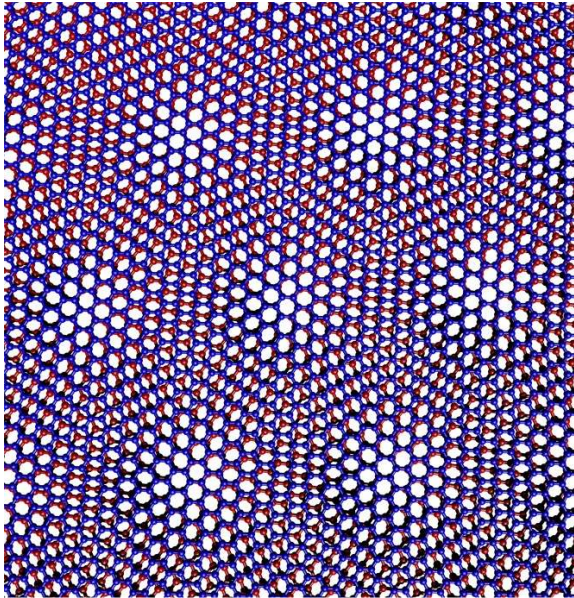


Science 361, 6403, 690–693 (2018)

These are unique features of two-dimensional materials

The tunability of twisted van der Waals materials

Twisted bilayer graphene

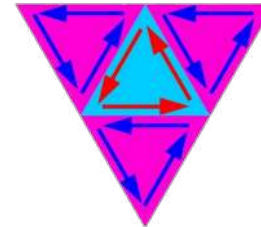


Superconductivity



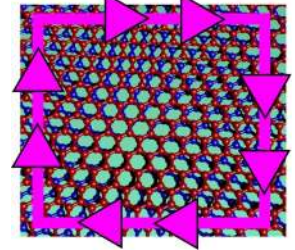
Nature 556, 43–50 (2018)

Topological networks



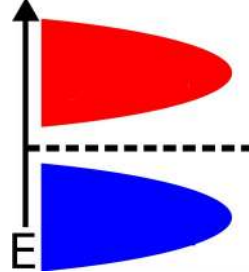
Nano Lett. 18, 11, 6725-6730 (2018)

Chern insulators



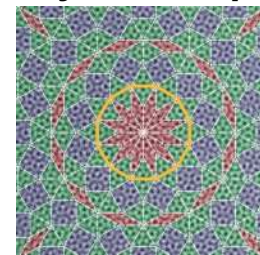
Science 365, 605-608 (2019)

Correlated insulators



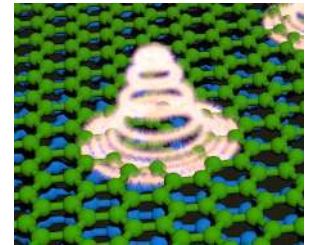
Nature 556, 80–84 (2018)

Quasicrystalline physics



Science 361, 782-786 (2018)

Proximal fractional Chern insulators

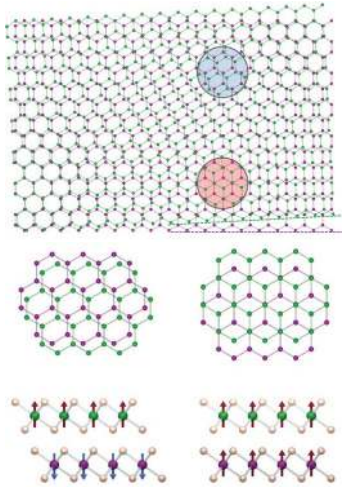


Nature 600, 439–443 (2021)

Twisted multilayers provide a powerful platform for emergent phenomena

Artificial quantum matter in moire van der Waals heterostructures

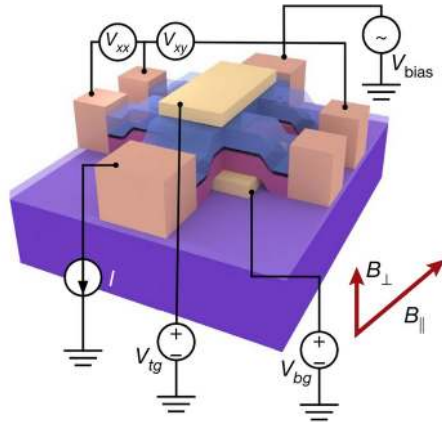
Unconventional magnets



Twisted CrBr_3

Science, 374(6571),
1140-1144 (2021)

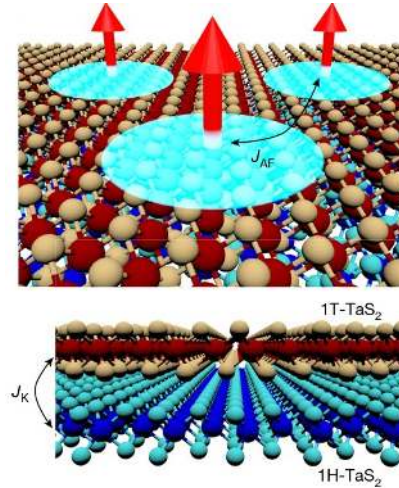
Unconventional superconductors



Twisted trilayer
graphene

Nature 595,
526–531 (2021)

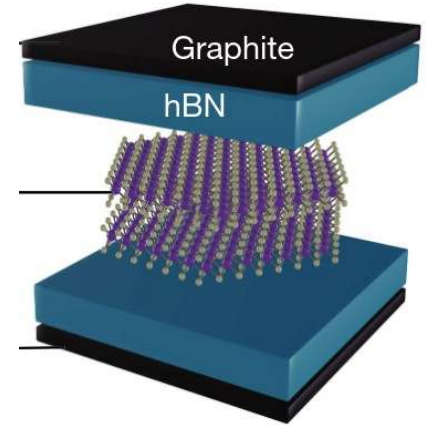
Heavy-fermion quantum materials



1H-1T TaS_2

Nature 599,
582–586 (2021)

Fractional topological matter

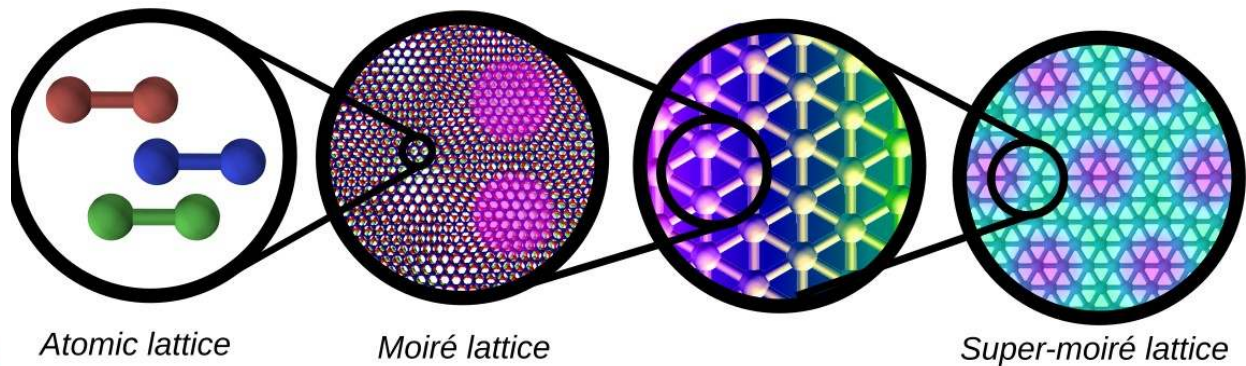
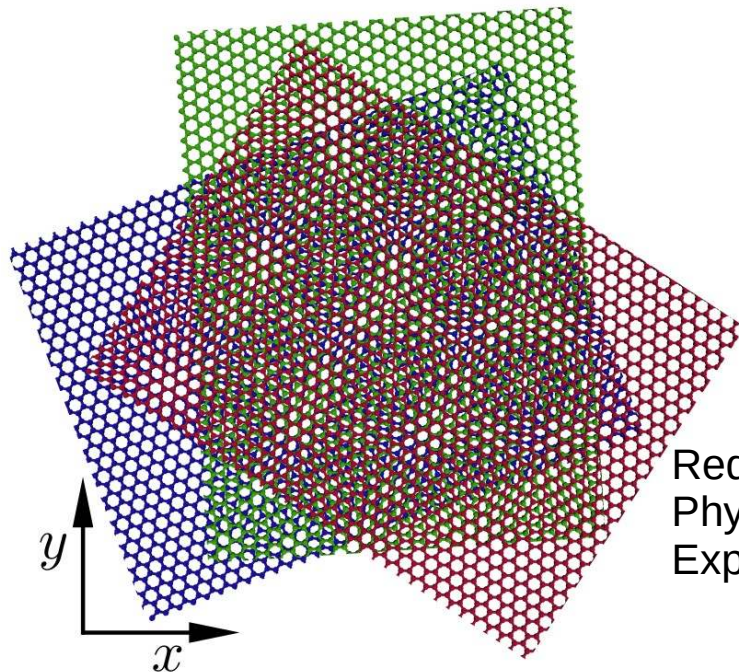


Twisted MoTe_2

Nature 622,
63–68 (2023)

Super-moire materials

Moire-of-moire materials



Requires computing up to a billion sites (10^9)
Physics at several length scales (atomic, moire, and super-moire)
Experiments showing correlations and unconventional superconductivity

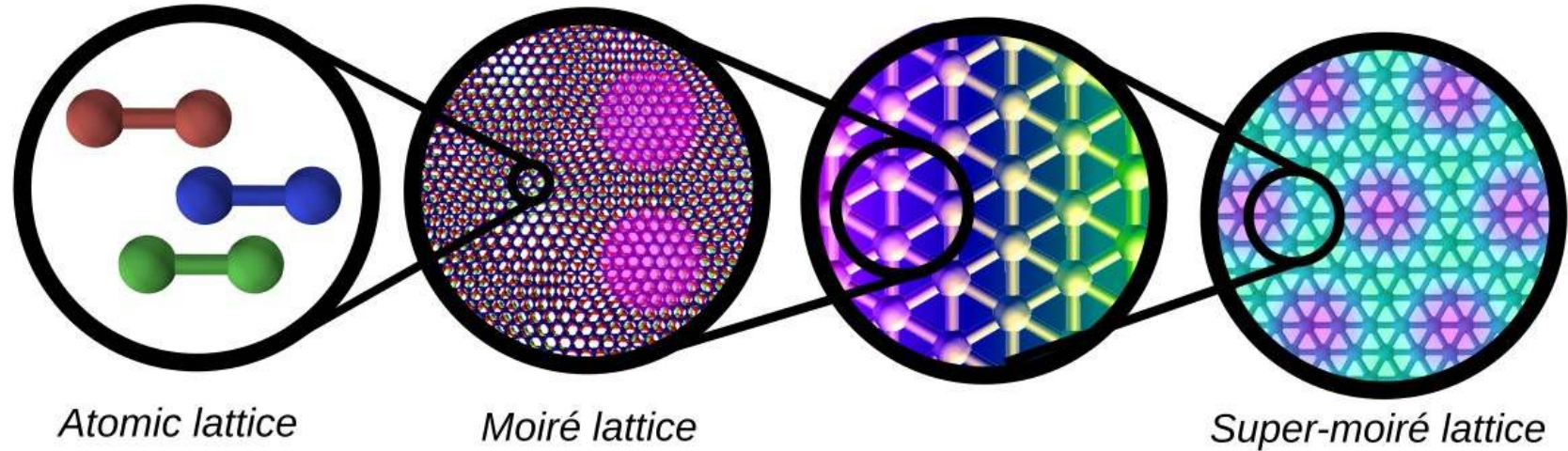
Nature 620, 762–767 (2023)

Nature 625, 494–499 (2024)

Nature 641, 896–903 (2025)

How can we compute the electronic structure of exceptionally large systems?

Why super-moire materials are hard (for theorists)



Moire systems **$N=10^5$ sites**, calculations taking around 1 minute

Computational cost grows as **N** (best case) or **N^3** (worst case)

Super-moire **$N=10^9$ sites**, calculations taking 10 days – 1000000 years

Is there a way to solve exceptionally large electronic structure problems?

(even going beyond usual memory limitations of conventional methods)

Behind the scenes

Yitao Sun



Tiago Antão



Marcel Niedermeier



Adolfo Fumega



Correlated states in super-moiré materials with a kernel polynomial quantics tensor cross interpolation algorithm, AO Fumega, M Niedermeier, JL Lado, **2D Materials 12 (1), 015018 (2025)**

Self-consistent tensor network method for correlated super-moire matter beyond one billion sites, Y Sun, M Niedermeier, TVC Antão, AO Fumega, JL Lado, **arXiv:2503.04373 (2025)**

Tensor network method for real-space topology in quasicrystal Chern mosaics, TVC Antão, Y Sun, AO Fumega, JL Lado, **arXiv:2506.05230 (2025)**

An exponential computational
challenge: quantum many.body

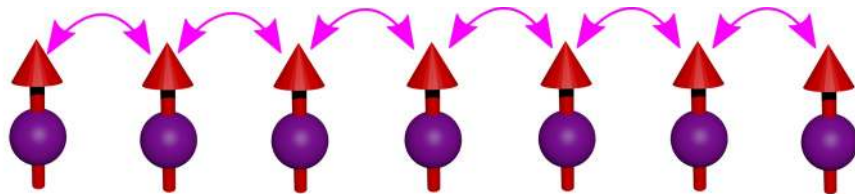
The problem of dimensionality

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 tight binding 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 take a simple many-body problem

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

And let us imagine that we have L different sites on our system and $S=1/2$

For example, for $L=2$ sites the elements of the basis are

$$|\uparrow\uparrow\rangle \quad |\uparrow\downarrow\rangle \quad |\downarrow\uparrow\rangle \quad |\downarrow\downarrow\rangle$$

For $L=3$ sites the elements of the basis are

$$\begin{array}{cccc} |\uparrow\uparrow\uparrow\rangle & |\uparrow\uparrow\downarrow\rangle & |\uparrow\downarrow\uparrow\rangle & |\uparrow\downarrow\downarrow\rangle \\ |\downarrow\uparrow\uparrow\rangle & |\downarrow\uparrow\downarrow\rangle & |\downarrow\downarrow\uparrow\rangle & |\downarrow\downarrow\downarrow\rangle \end{array}$$

The quantum many-body problem

Let us take a simple many-body problem

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

And let us imagine that we have L different sites on our system and $S=1/2$

For $L=4$ sites, the elements of the basis are

$ \uparrow\uparrow\uparrow\uparrow\rangle$	$ \uparrow\uparrow\uparrow\downarrow\rangle$	$ \uparrow\uparrow\downarrow\uparrow\rangle$	$ \uparrow\uparrow\downarrow\downarrow\rangle$
$ \uparrow\downarrow\uparrow\uparrow\rangle$	$ \uparrow\downarrow\uparrow\downarrow\rangle$	$ \uparrow\downarrow\downarrow\uparrow\rangle$	$ \uparrow\downarrow\downarrow\downarrow\rangle$
$ \downarrow\uparrow\uparrow\uparrow\rangle$	$ \downarrow\uparrow\uparrow\downarrow\rangle$	$ \downarrow\uparrow\downarrow\uparrow\rangle$	$ \downarrow\uparrow\downarrow\downarrow\rangle$
$ \downarrow\downarrow\uparrow\uparrow\rangle$	$ \downarrow\downarrow\uparrow\downarrow\rangle$	$ \downarrow\downarrow\downarrow\uparrow\rangle$	$ \downarrow\downarrow\downarrow\downarrow\rangle$

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

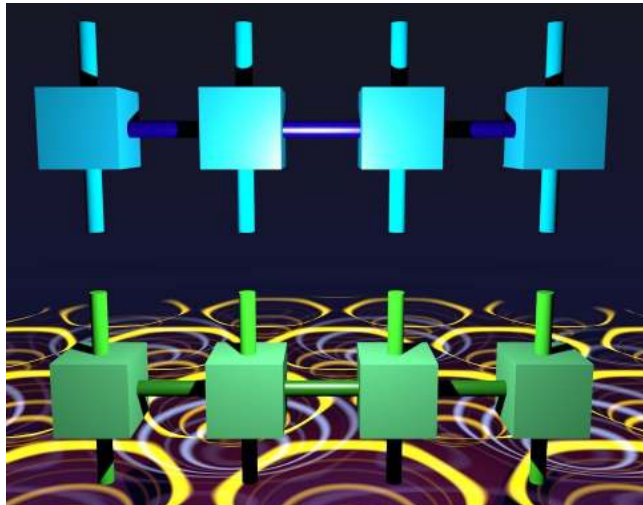
Is there an efficient way of storing so many coefficients?

Dealing with exponentially large spaces: the quantum many-body problem

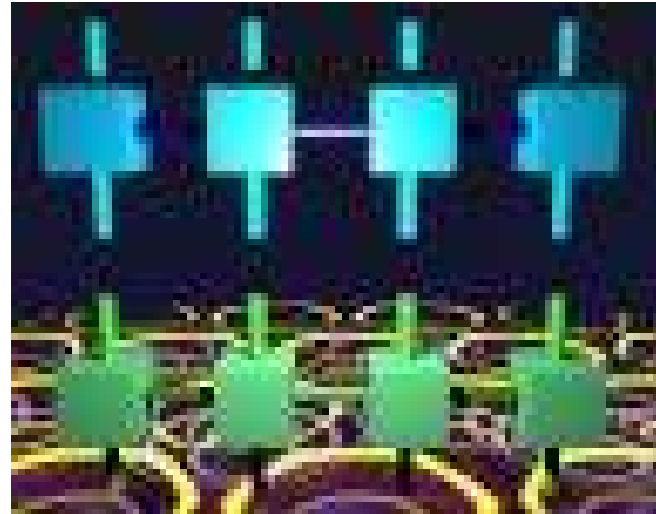
A many-body wavefunction is a very high dimensional object (2^L coefficients)

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

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



“True wavefunction”



“Tensor-network wavefunction”

The matrix-product state ansatz

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

Let us imagine to propose a parametrization in this form

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

dimension 2^L dimension $\sim Lm^2$

(m dimension of the matrix)

State compression with tensor-networks

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

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



Matrix product state

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

Dealing with exponentially large spaces: the quantum many-body problem

Typical many-body wavefunction $|\Psi\rangle = \sum c_{s_1, s_2, \dots, s_L} |s_1, s_2, \dots, s_L\rangle$

We need to determine in total 2^L coefficients

Is there an efficient way of storing so many coefficients?

Tensor networks allow parametrizing many-body wavefunctions as

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

$L\chi^2$ parameters

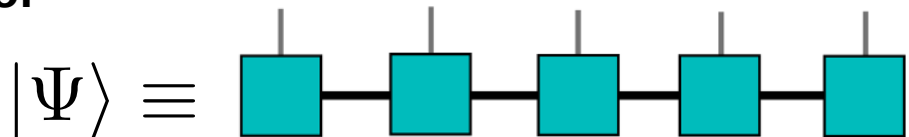


Tensor networks allow to drastically reduce the memory required to store a many-body state

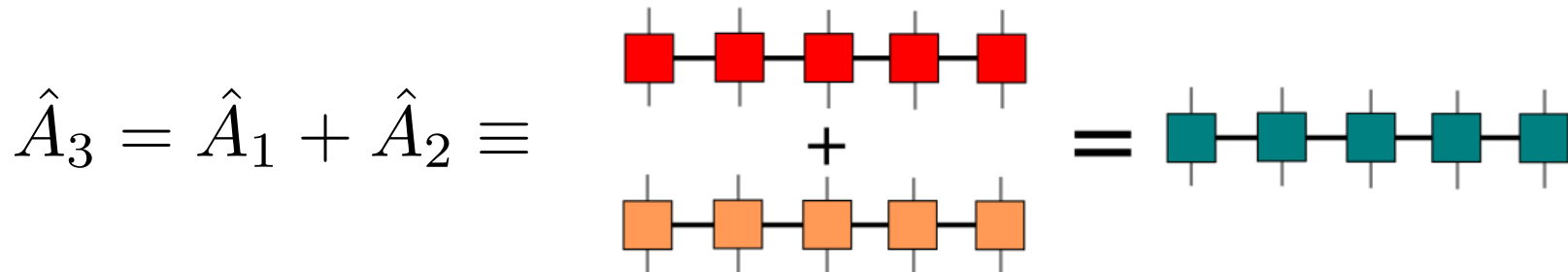
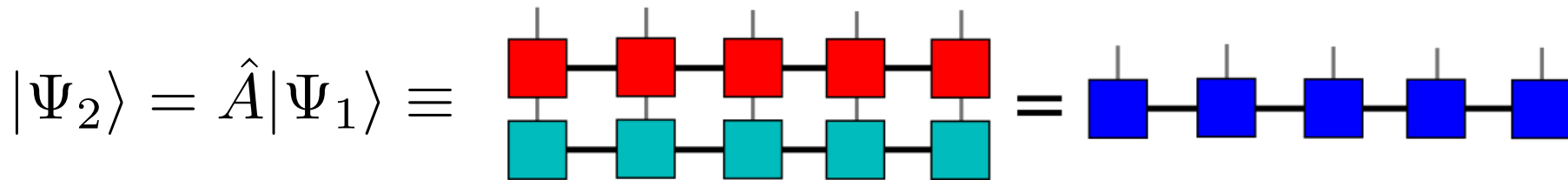
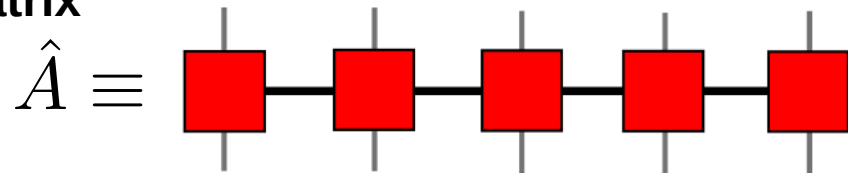
Exponentially large algebra with tensor networks

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

vector

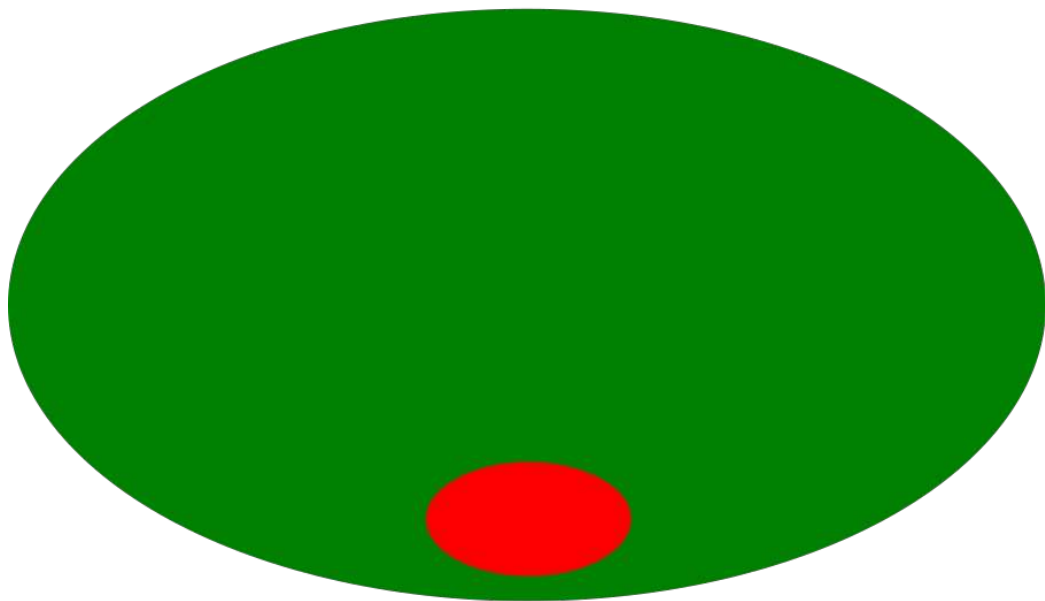


matrix



MPS as a parametrization of finite entanglement states

Full Hilbert space



Tensor network states

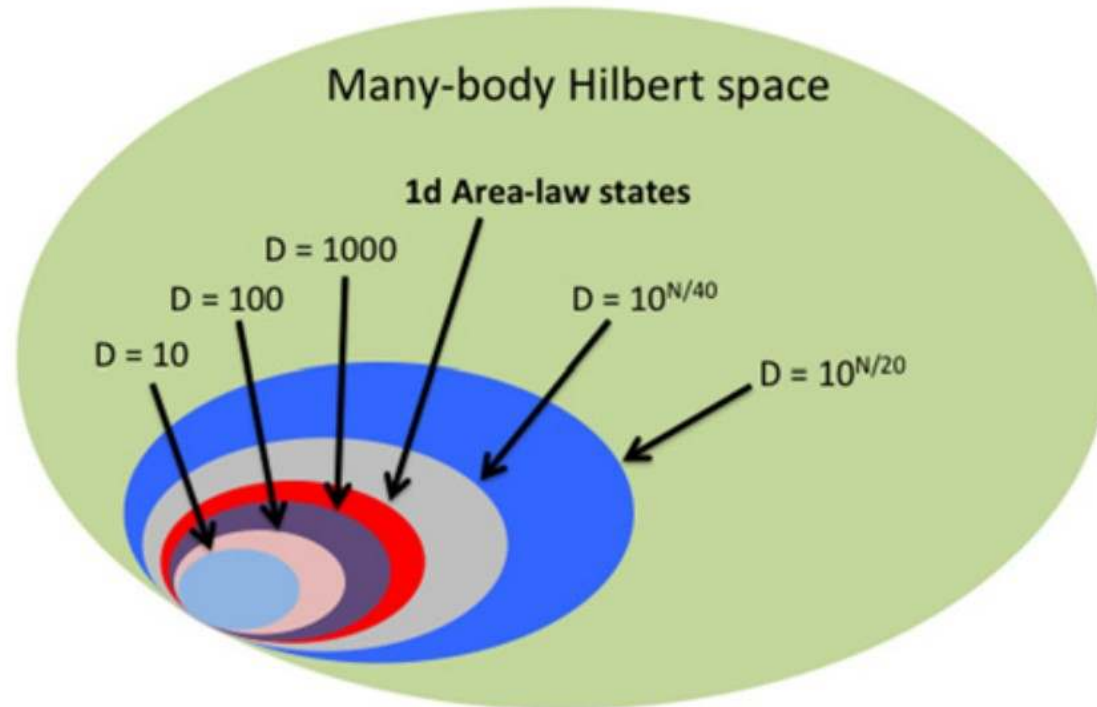
$$c_{s_1, s_2, \dots, s_L} = M_1^{s_1} M_2^{s_2} \dots M_L^{s_L}$$

MPS have an entanglement entropy
bounded by the bond dimension

$$S \sim \log(m)$$

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 many-body problems have ground states that can be captured with this ansatz

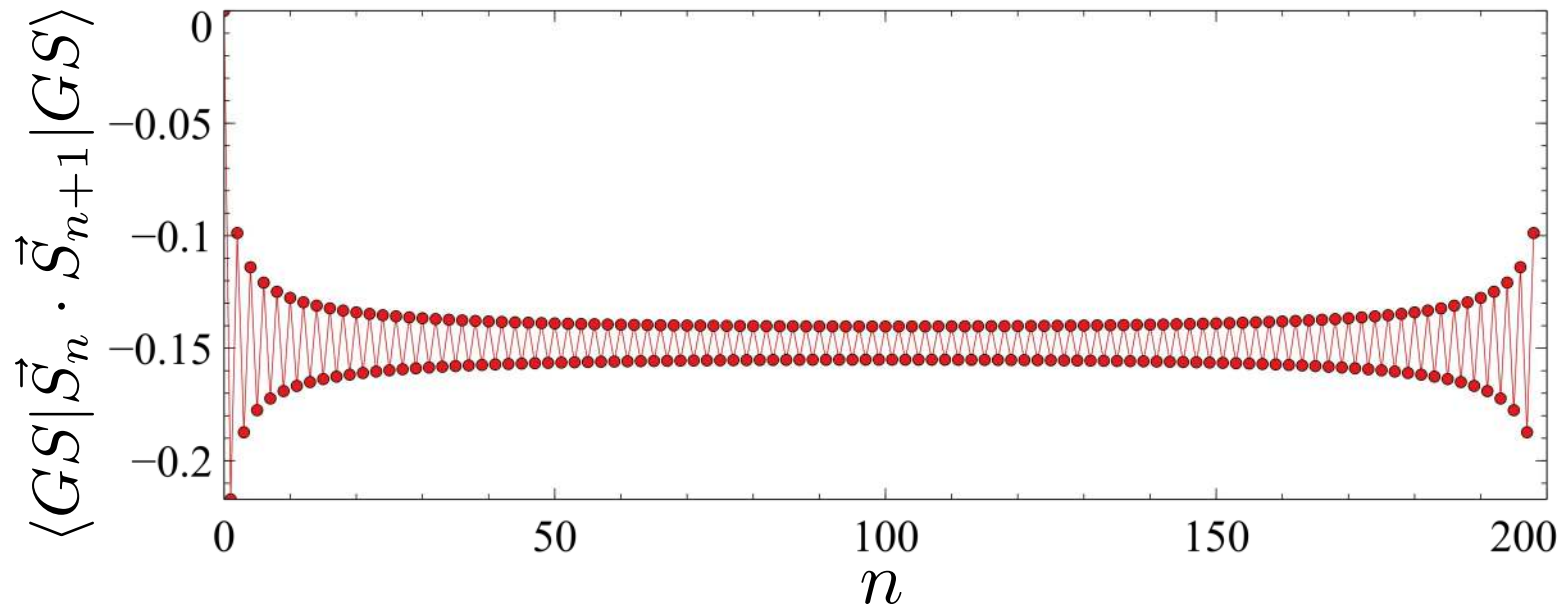
$$c_{s_1, s_2, \dots, s_L} = M_1^{s_1} M_2^{s_2} \dots M_L^{s_L}$$

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

The Heisenberg model with tensor-networks

Non-uniform Heisenberg model

$$\mathcal{H} = \sum_n J(n) \vec{S}_n \cdot \vec{S}_{n+1}$$
$$J(n) = J_0 + \delta \cos \Omega n$$

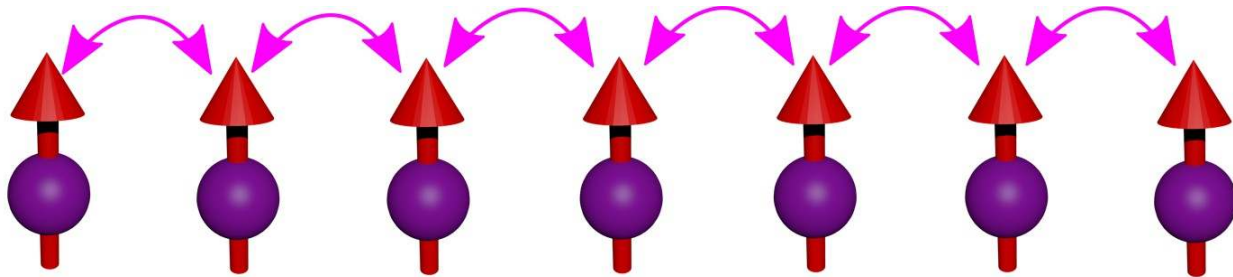


Tensor networks allow solving a 200 many-body spin model in a few seconds in a laptop

Many-body dynamical correlators

One dimensional Heisenberg Hamiltonian

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

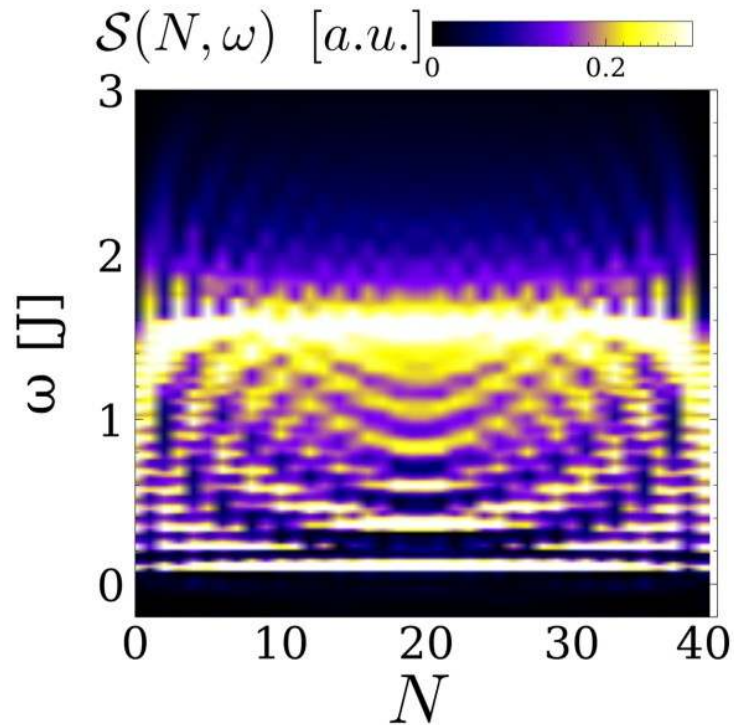


Tensor networks allow computing dynamical correlators

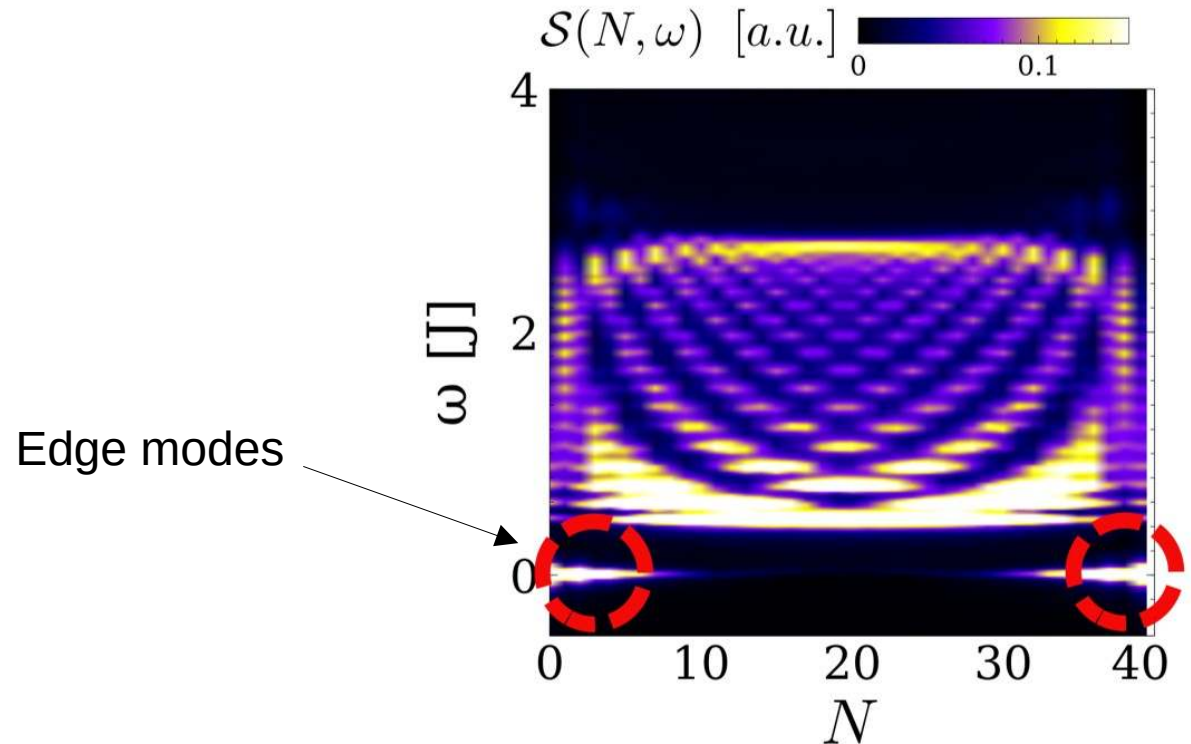
$$\mathcal{S}(N, \omega) = \langle GS | S_N^z \delta(\omega - \mathcal{H} + E_0) S_N^z | GS \rangle$$

Dynamical structure factor of a Heisenberg model

S=1/2 chain

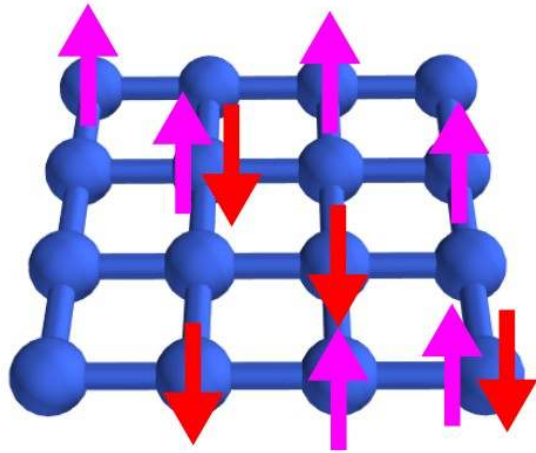


S=1 chain



Some paradigmatic problems solved with matrix product states

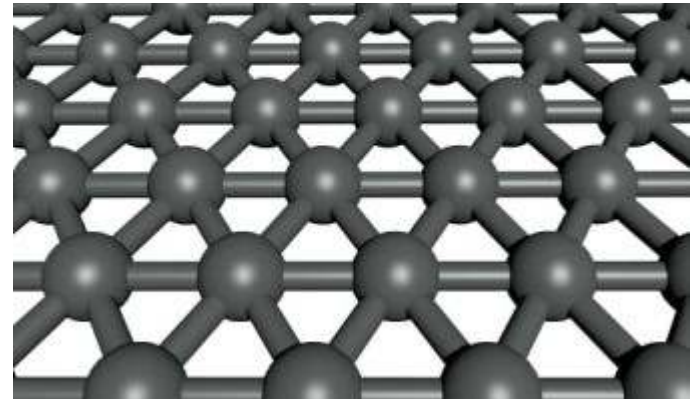
Solving the 2D Hubbard model at finite doping



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

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

Solving the 2D Heisenberg model in frustrated lattices

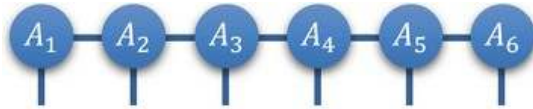


$$\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

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

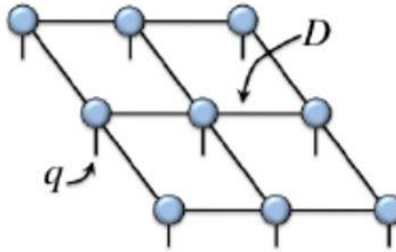
Many-body state compression

Matrix-product states



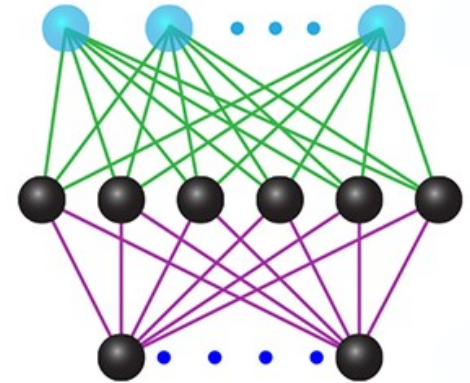
Phys. Rev. Lett. 69, 2863 (1992)

Projected entangled pair-states



Annals of Physics 326, 96 (2011)

Neural-network quantum states

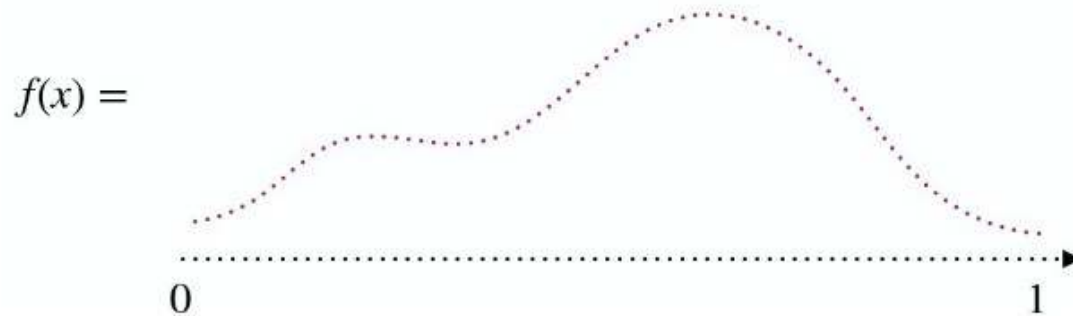


Science 355.6325 (2017): 602-606.

Other compressed many-body states could be potentially used for exponentially large problems

Tensor networks for non quantum-many body

Imagine that you have a function with an exponentially large number of points



We could store all those values with a tensor network

$$c_{s_1, s_2, \dots, s_L} = M^{s_1} M^{s_2} \dots M^{s_L}$$

$$x = \sum_n 2^{-n} s_n \quad f(x) = c_{s_1, s_2, \dots, s_L} \quad s_n = 0, 1$$

There is an algorithm (tensor cross interpolation) that enables to systematically build the MPS

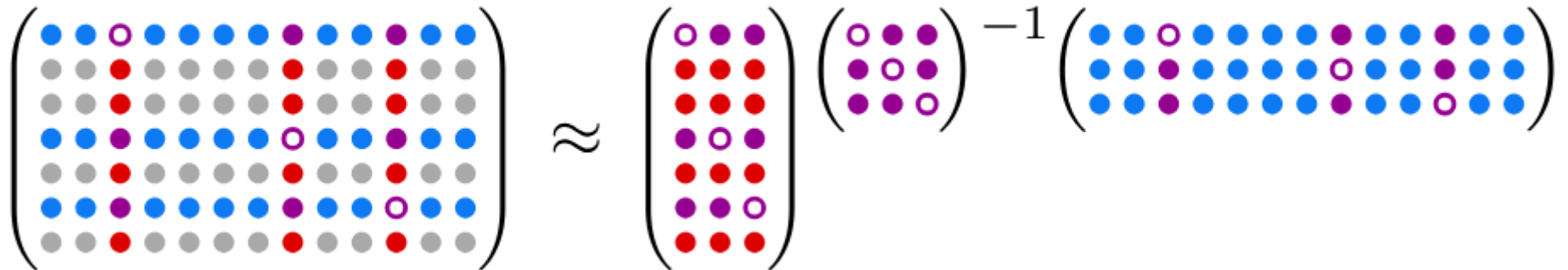
Quantum-inspired active learning algorithm

Machine learning tensor networks

How do we learn the tensor network representation of an exponentially large object?

With a cross interpolation algorithm with the tensor network

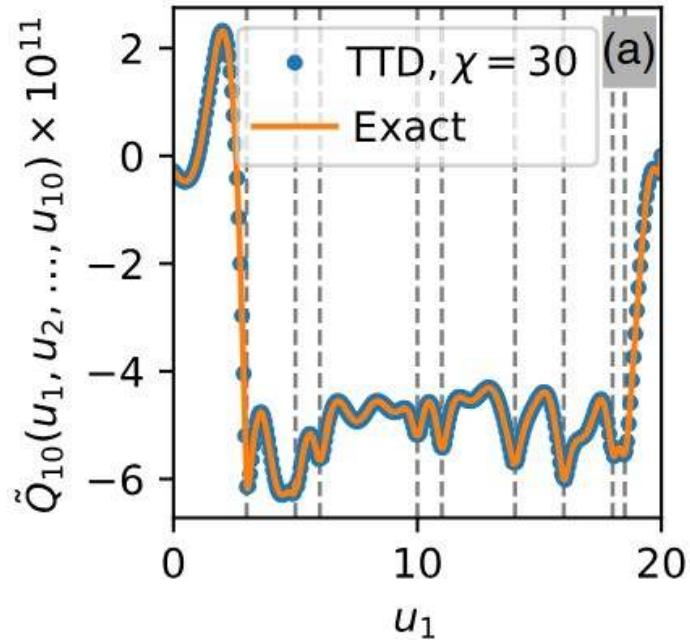
$$A \approx CP^{-1}R = \tilde{A}$$


$$\left(\begin{array}{cccccccccccc} \bullet & \bullet & \circ & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \end{array} \right) \approx \left(\begin{array}{ccc} \circ & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \end{array} \right) \left(\begin{array}{ccc} \circ & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \end{array} \right)^{-1} \left(\begin{array}{cccccccccccc} \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \end{array} \right)$$

Quantum inspired active learning to learn exponentially large spaces

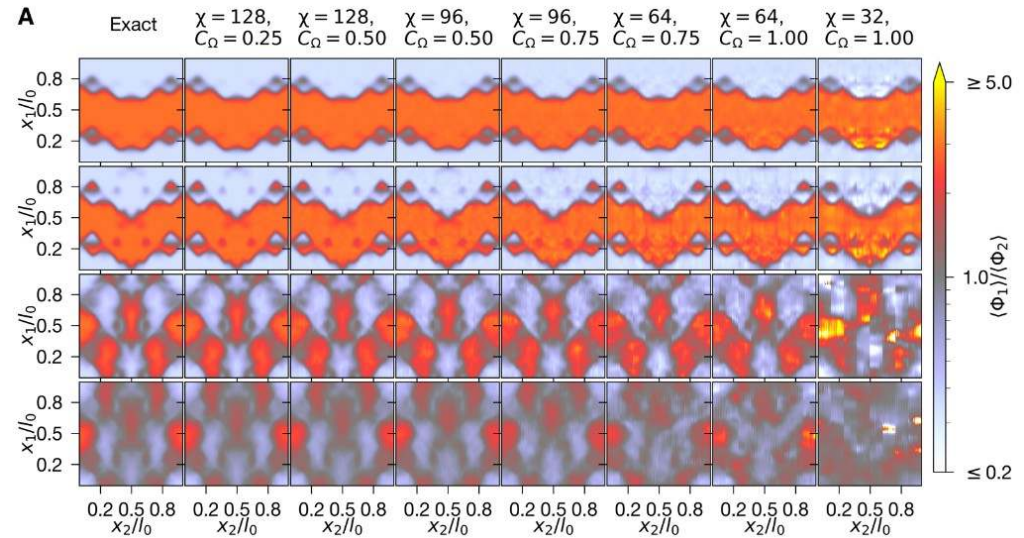
Learning exponentially large spaces with tensor networks

High dimensional integrals for Feynman diagrams



Phys. Rev. X 12, 041018 (2022)

Probabilistic turbulence distributions



Science Advances, 11 (5) 2025

Tensor networks for interacting super-moire materials

The challenge of correlated super-moire materials

Hamiltonian describing electrons in a super-moire material

$$H = H_0 + H_V = \sum_{\alpha\beta} t_{\alpha\beta} c_{\alpha}^{\dagger} c_{\beta} + \sum_{\alpha\beta} V_{\alpha\beta} c_{\alpha}^{\dagger} c_{\alpha} c_{\beta}^{\dagger} c_{\beta}$$

Mean-field treatment of the interacting Hamiltonian

$$H^{MF} = \sum_{\alpha\beta} (t_{\alpha\beta} + \chi_{\alpha\beta}) c_{\alpha}^{\dagger} c_{\beta} = \sum_{\alpha\beta} H_{\alpha\beta}^{MF} c_{\alpha}^{\dagger} c_{\beta}$$

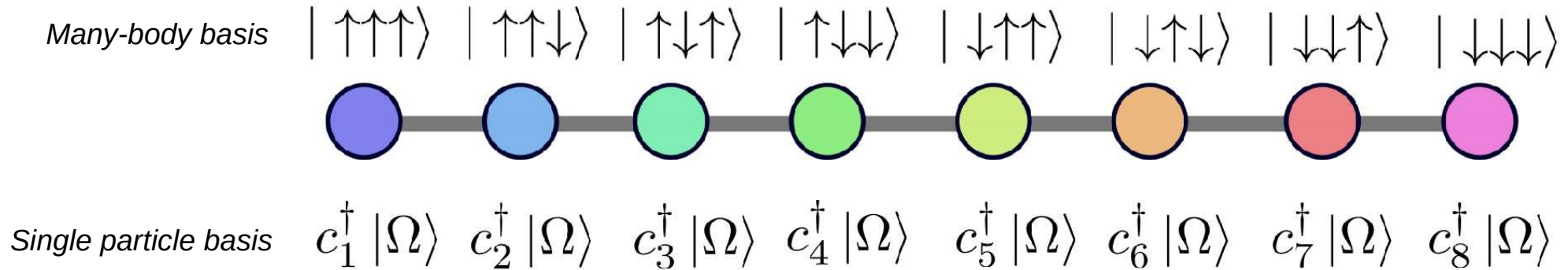
Solving the system requires dealing with matrices proportional to the system size

In a super-moire system, this requires solving a billion sites

How could we solve a system whose Hamiltonian would be too large to store?
(even before considering the time required to solve it)

Tensor network machine learning for single particle problems

We can identify a many-body space with a very large single particle one



We can use a many-body method (tensor-networks) to solve an exponentially large problem

2D Materials 12 (1), 015018 (2025)

arXiv:2503.04373 (2025)

How can we build this compressed representation for an exponentially large object?

*With quantics tensor-cross interpolation: **a quantum-inspired active learning algorithm***

Phys. Rev. Lett. 132, 056501 (2024)

SciPost Phys. 18, 104 (2025)

Self-consistent electronic interactions with tensor networks

We represent the super-moire electronic Hamiltonian as a tensor-network

$$\mathcal{H}_{\alpha\beta}^{MF} \equiv \Gamma_{s_1, s'_1}^{(1)} \Gamma_{s_2, s'_2}^{(2)} \Gamma_{s_3, s'_3}^{(3)} \dots \Gamma_{s_L, s'_L}^{(L)} \quad \mathcal{H}_{\alpha\beta}^{MF} \equiv \text{[Diagram: A sequence of orange squares connected horizontally, representing a tensor network.]}$$

The mean-field problem can be reformulated purely with tensor networks

Tensor Network SCF loop

$$\begin{aligned} \mathcal{H}_{\alpha\beta}^{MF} &\equiv \text{[Diagram: A sequence of orange squares connected horizontally, representing a tensor network.]} = t_{\alpha\beta} + \chi_{\alpha\beta} \left(\text{[Diagram: A sequence of cyan squares connected horizontally, representing a tensor network.]} \right) \\ \langle c_{\alpha}^{\dagger} c_{\beta} \rangle &\equiv \text{[Diagram: A sequence of cyan squares connected horizontally, representing a tensor network.]} = \sum_n \lambda_n T_n \left(\text{[Diagram: A sequence of orange squares connected horizontally, representing a tensor network.]} \right) \end{aligned}$$

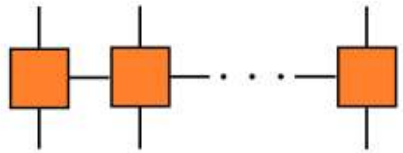
Self-consistent electronic interactions with tensor networks

Super-moire interacting Hamiltonian

$$H = H_0 + H_V = \sum_{\alpha\beta} t_{\alpha\beta} c_{\alpha}^{\dagger} c_{\beta} + \sum_{\alpha\beta} V_{\alpha\beta} c_{\alpha}^{\dagger} c_{\alpha} c_{\beta}^{\dagger} c_{\beta}$$

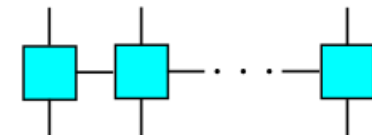
Mean-field decoupled Hamiltonian

$$H^{MF} = \sum_{\alpha\beta} (t_{\alpha\beta} + \chi_{\alpha\beta}) c_{\alpha}^{\dagger} c_{\beta} = \sum_{\alpha\beta} H_{\alpha\beta}^{MF} c_{\alpha}^{\dagger} c_{\beta}$$

$$\mathcal{H}_{\alpha\beta}^{MF} \equiv \text{---} \text{---} \text{---} \text{---} \text{---} \text{---}$$


A diagram representing the mean-field decoupled Hamiltonian as a 1D chain of orange squares. Each square has a vertical line passing through its center, and they are connected by horizontal lines. Ellipses between the first and second squares, and between the last two squares, indicate an infinite chain.

Chebyshev expansion of the correlators

$$\langle c_{\alpha}^{\dagger} c_{\beta} \rangle = \langle \alpha | \Xi(\mathcal{H}^{MF}) | \beta \rangle \equiv \text{---} \text{---} \text{---} \text{---} \text{---} \text{---}$$


A diagram representing the Chebyshev expansion of the correlators as a 1D chain of cyan squares. Each square has a vertical line passing through its center, and they are connected by horizontal lines. Ellipses between the first and second squares, and between the last two squares, indicate an infinite chain.

$$\Xi(\mathcal{H}^{MF}) = \sum \lambda_n T_n(\mathcal{H}^{MF})$$

$$T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x)$$

Rev. Mod. Phys. 78, 275 (2006)
arXiv:2503.04373 (2025)

Spectral functions with tensor networks

Local spectral function of the mean-field Hamiltonian

$$D(\omega, \alpha) = \langle \alpha | \left[\sum_n T_n(\mathcal{H}^{MF}) P_n(\omega) \right] | \alpha \rangle$$

With a tensor network Chebyshev algorithm

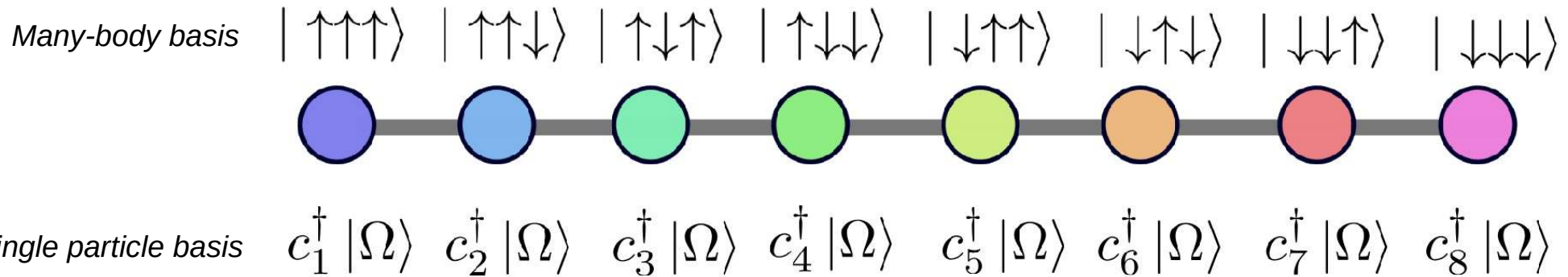
$$P_n(\omega) = \frac{2T_n(\omega)}{\pi\sqrt{1-\omega^2}}$$

$$T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x)$$

$$\mathcal{H}_{\alpha\beta}^{MF} \equiv \begin{array}{c} | \\ \text{[orange box]} \\ | \end{array} - \begin{array}{c} | \\ \text{[orange box]} \\ | \end{array} - \dots - \begin{array}{c} | \\ \text{[orange box]} \\ | \end{array}$$

Tensor network representation of a super-morrie Hamiltonian

We can identify a many-body space with a very large single particle one



In the tight binding basis uniform hopping takes the form

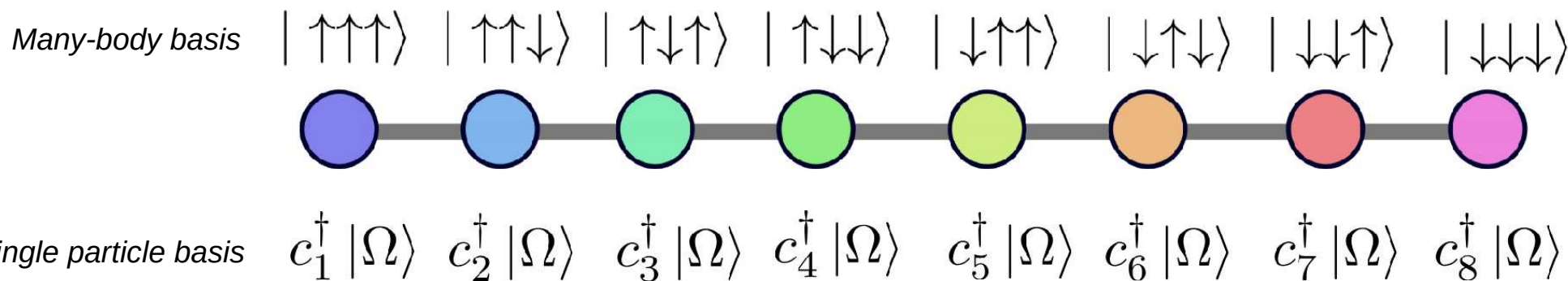
$$H_{0,NN} = \sum_{\alpha,s}^{N-1} t(c_{x_{\alpha+1},s}^\dagger c_{x_{\alpha},s} + h.c.)$$

In the tensor-network pseudospin basis, uniform hopping takes the form

$$\mathcal{H}_{0,NN} = \sum_{l,s}^L t(\sigma_{l,s}^+ \otimes_{m>l} \sigma_{m,s}^- + h.c.)$$

Tensor network representation of a super-moire Hamiltonian

We can identify a many-body space with a very large single particle one



The tensor-network moire hopping can be built as

Find the MPS representation for the modulation and store in a diagonal MPO $\mathcal{T}$

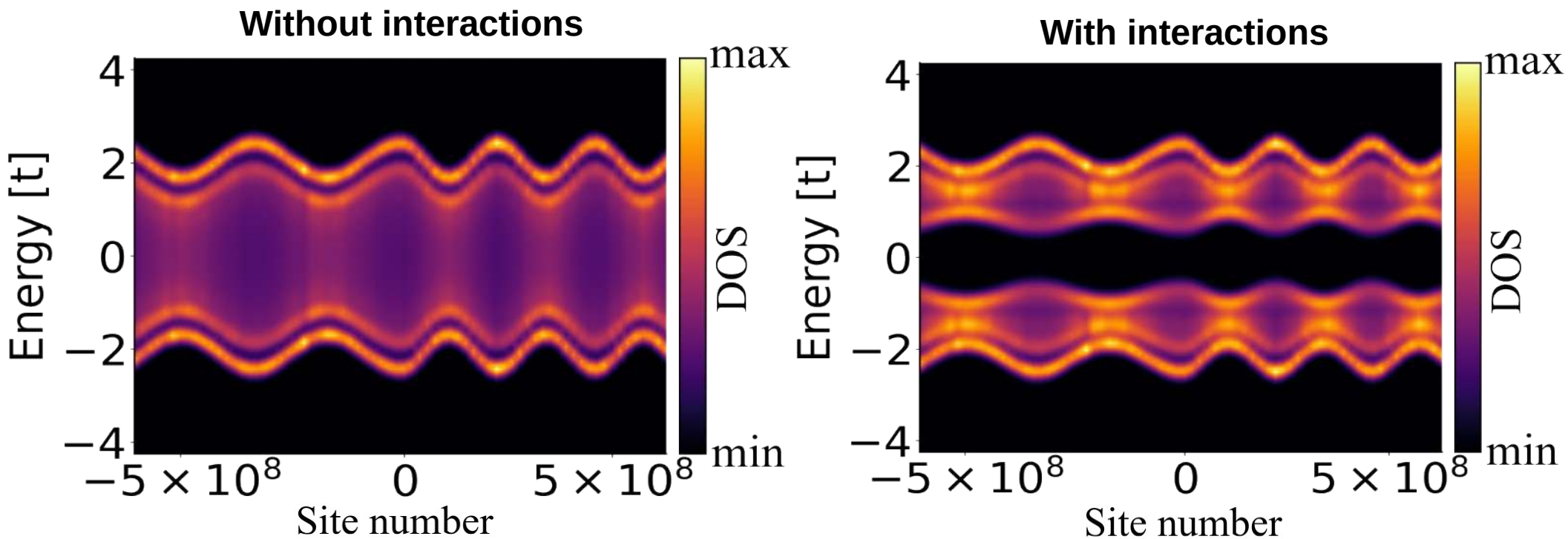
$$|\tau\rangle = \sum M_{s_1}^{(1)} M_{s_2}^{(2)} M_{s_3}^{(3)} \dots M_{s_L}^{(L)} |s_1, s_2, \dots, s_L\rangle$$

Quantics tensor cross interpolation

Modulated super-moire by construction

$$\mathcal{H}_0 = \{[\mathcal{T} \sum_{l,s}^L (\sigma_{l,s}^+ \otimes_{m>l} \sigma_{m,s}^-)] + h.c.\}$$

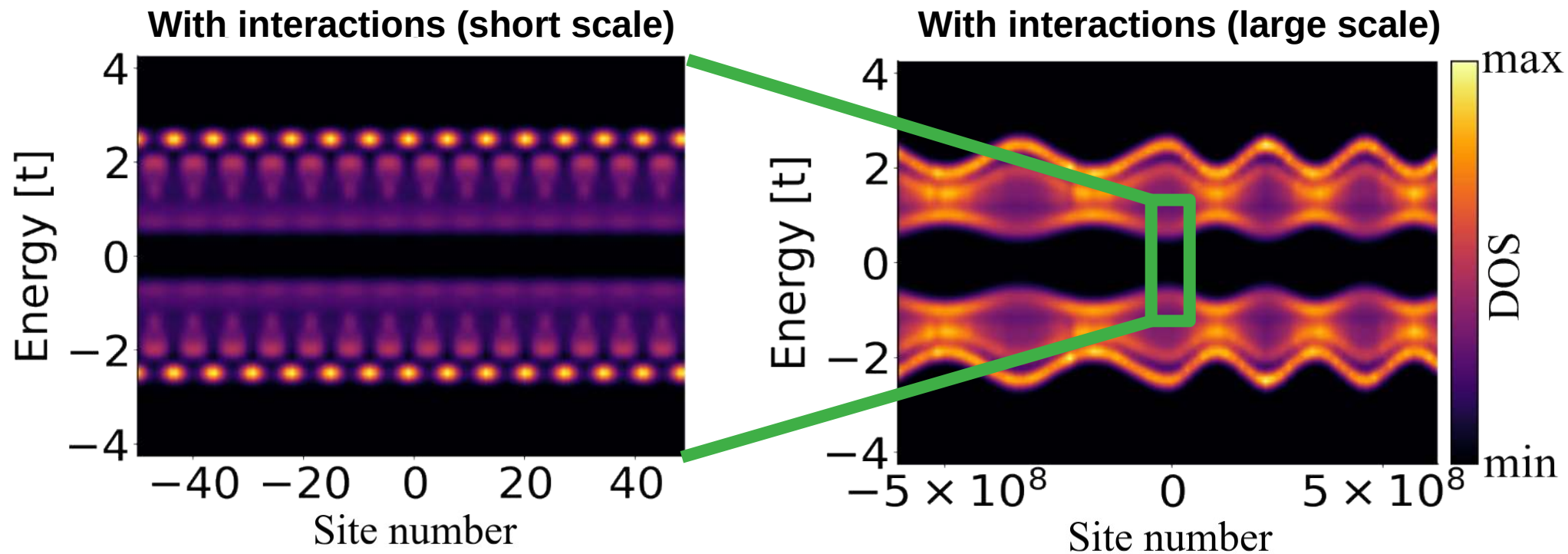
Solving billion-size super-moire materials



Tensor networks allow to solve selfconsistently a super-moire with one billion sites

arXiv:2503.04373 (2025)

Solving billion-size super-moire materials

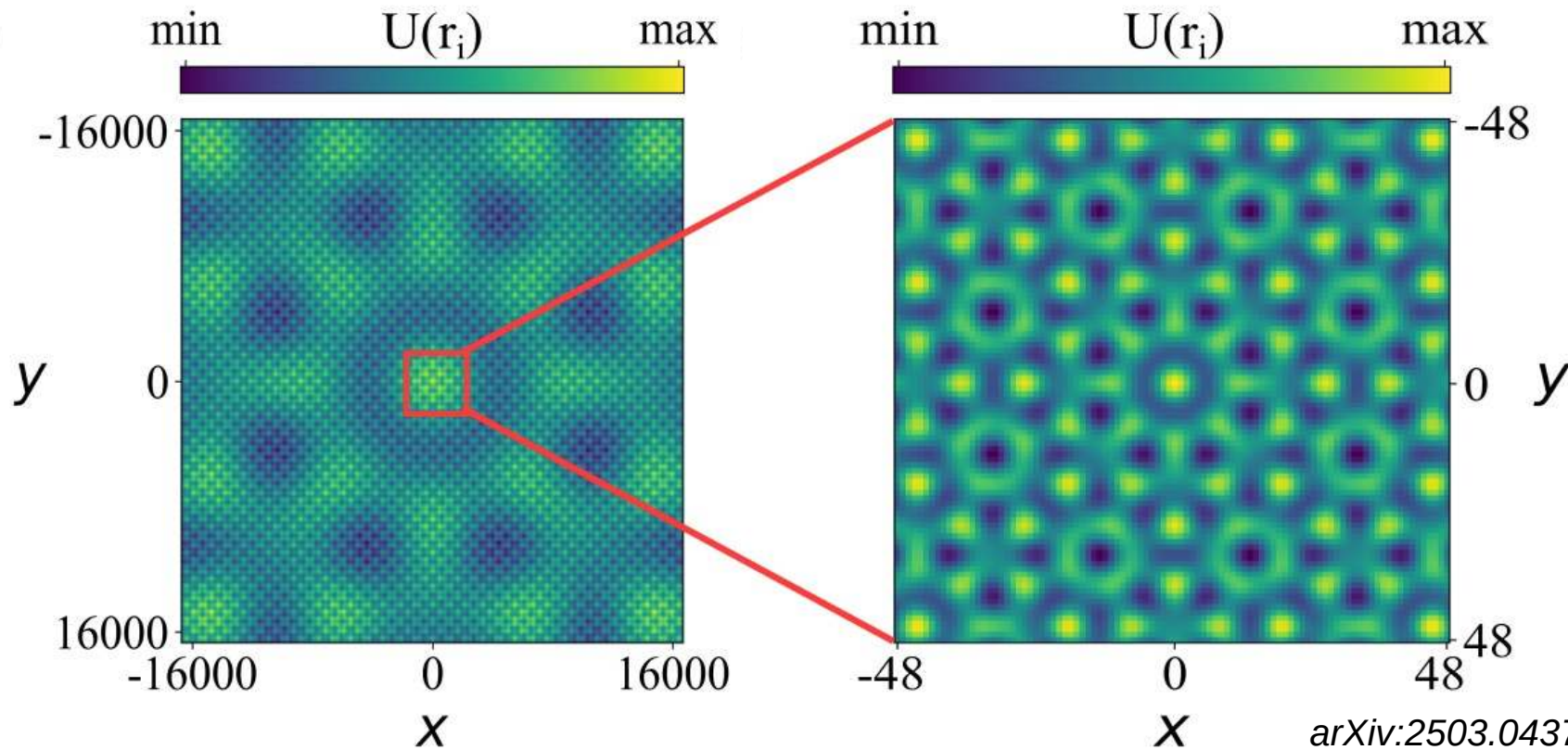


Tensor networks allow to solve selfconsistently a super-moire with one billion sites

arXiv:2503.04373 (2025)

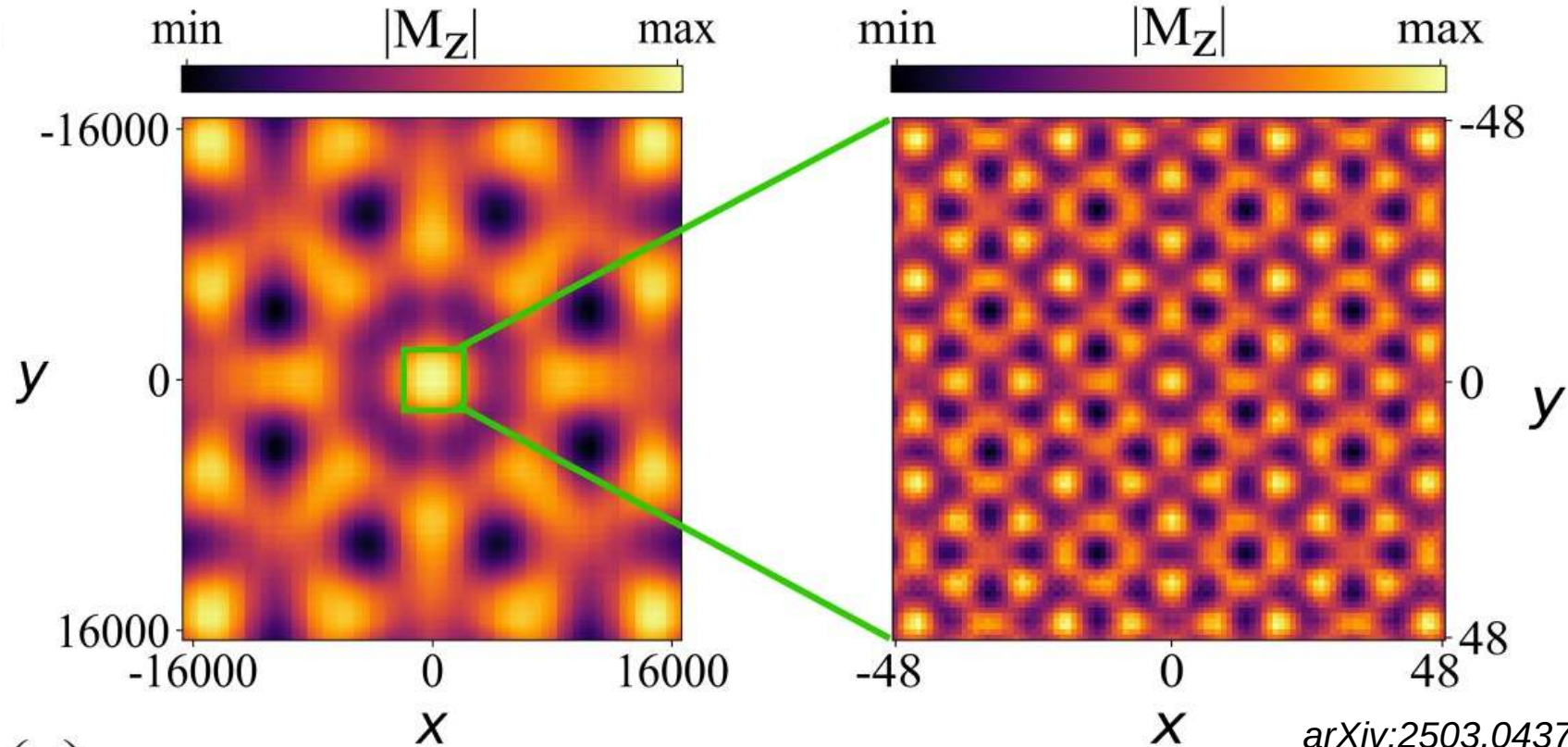
Two-dimensional billion size interacting super-moire

Modulation fo the Hamiltonian



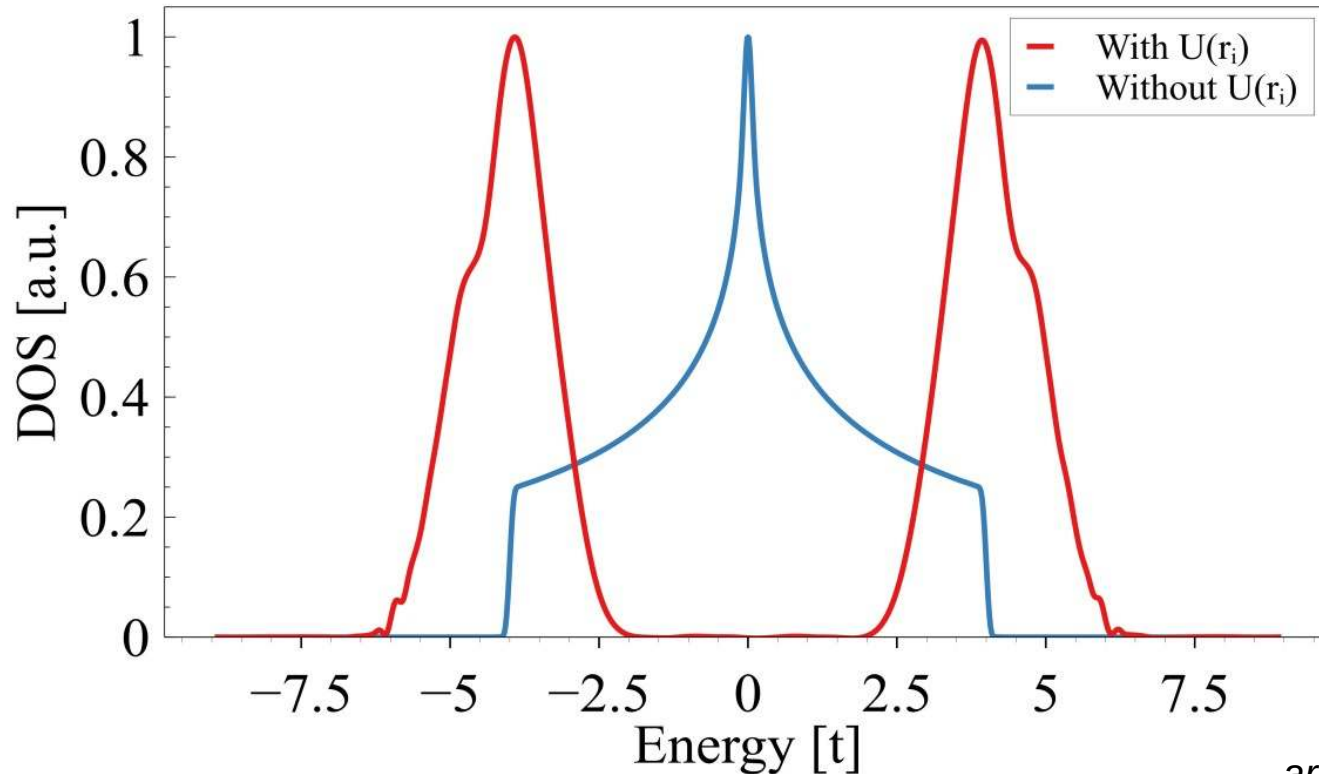
Two-dimensional billion size interacting super-moire

Selfconsistent symmetry broken order (magnetization)



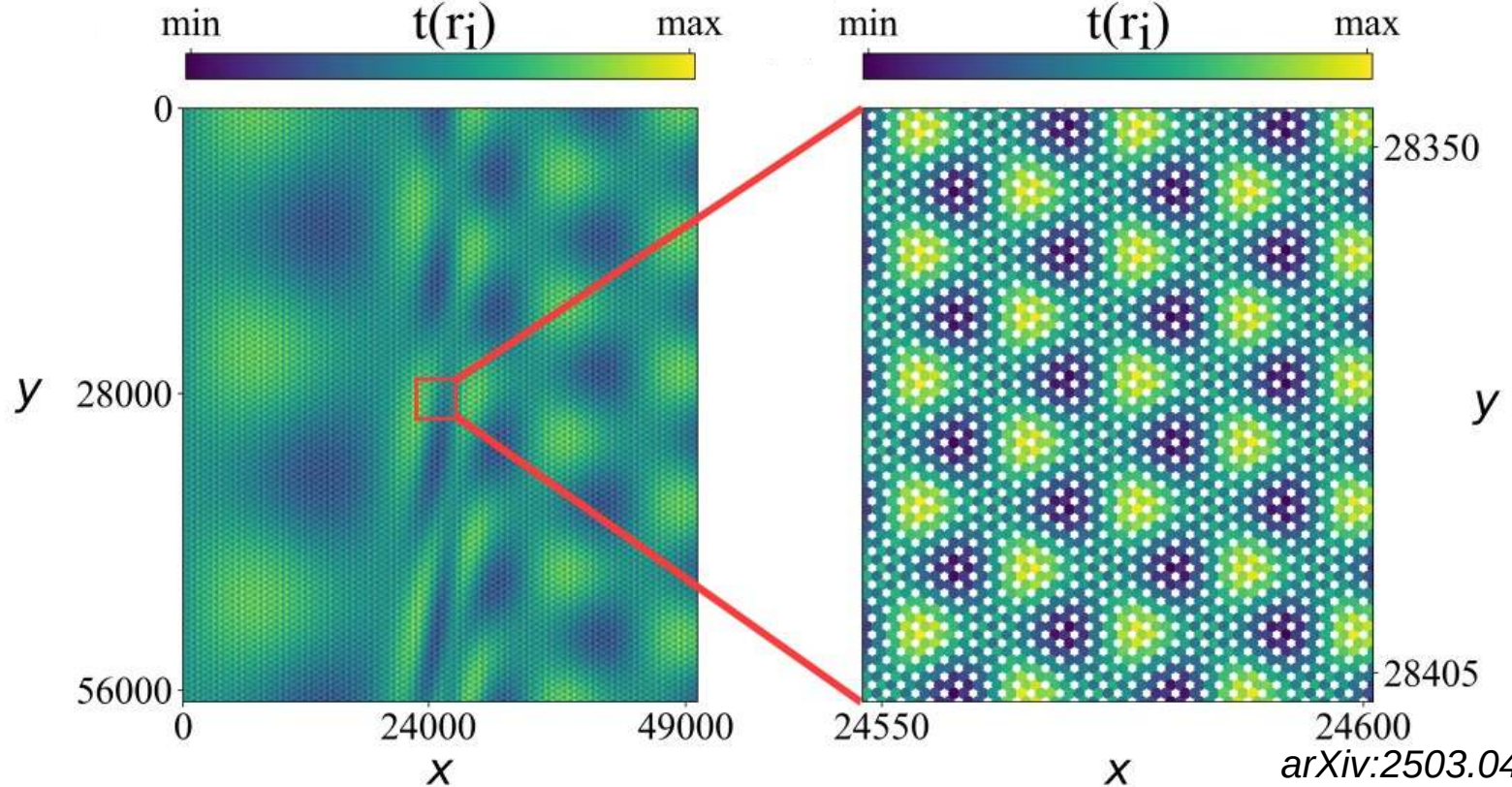
Two-dimensional billion size interacting super-moire

Spectral function with and without interactions



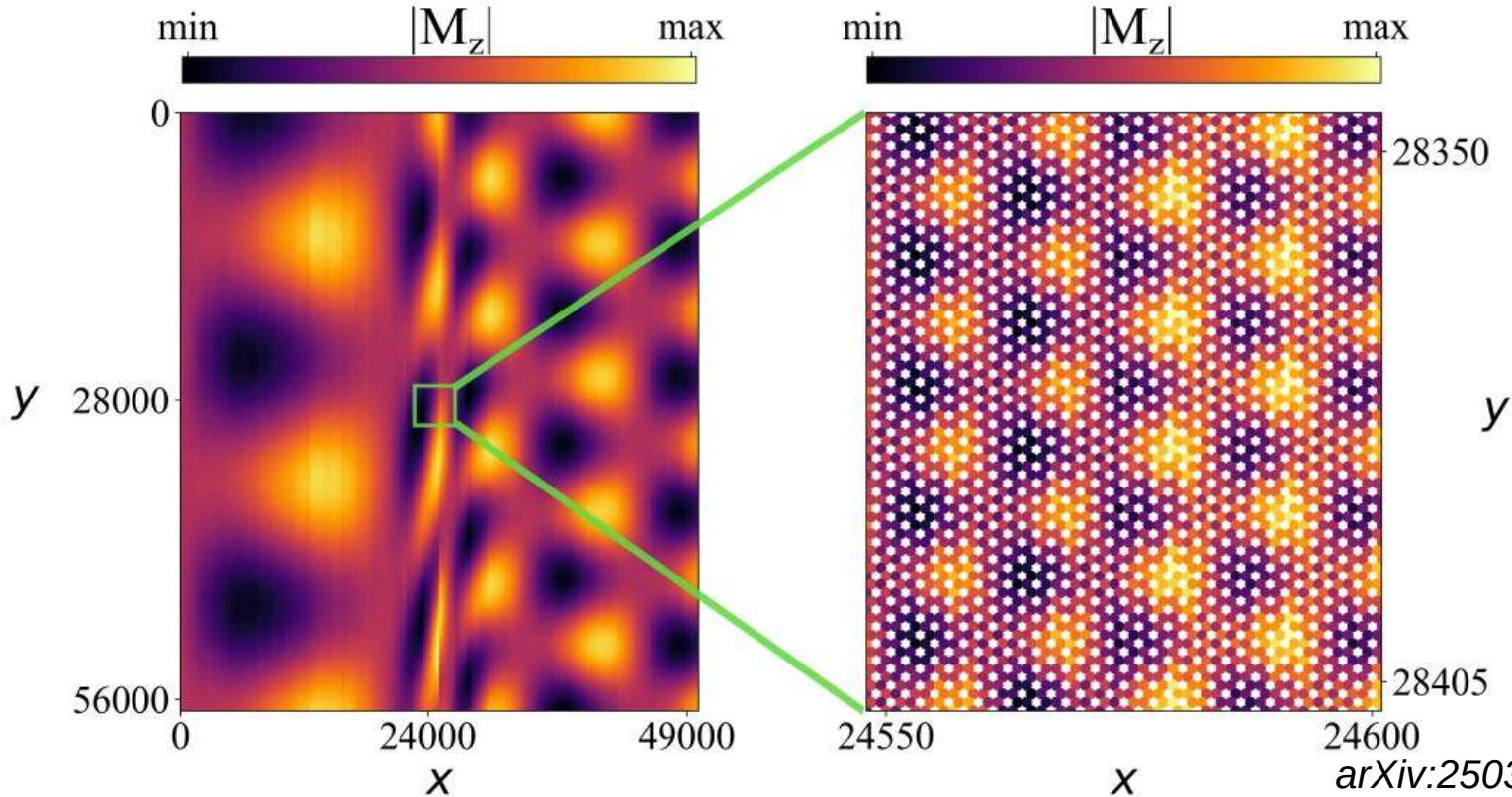
Two-dimensional billion size interacting super-moire

Modulation fo the Hamiltonian



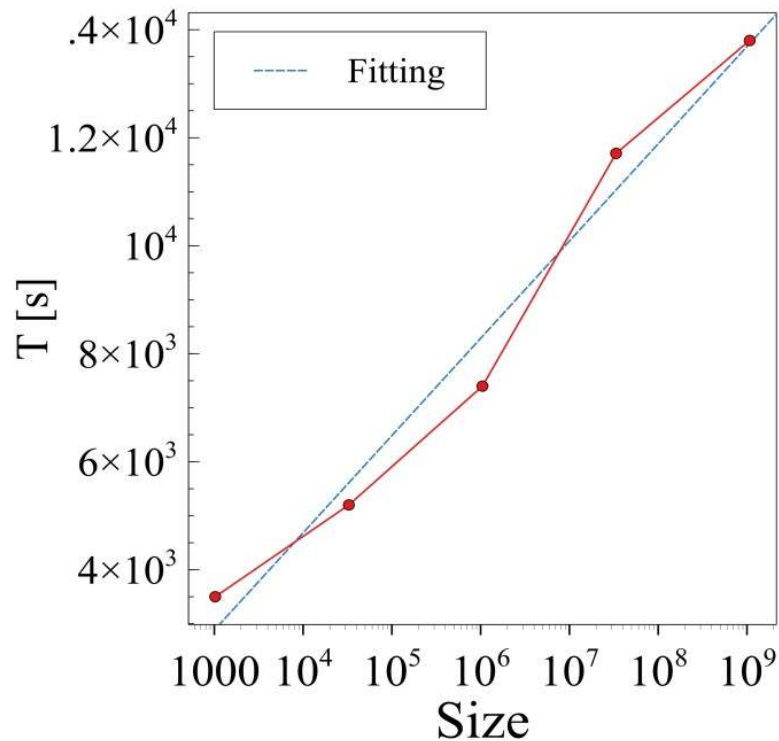
Two-dimensional billion size interacting super-moire

Selfconsistent symmetry broken order (magnetization)

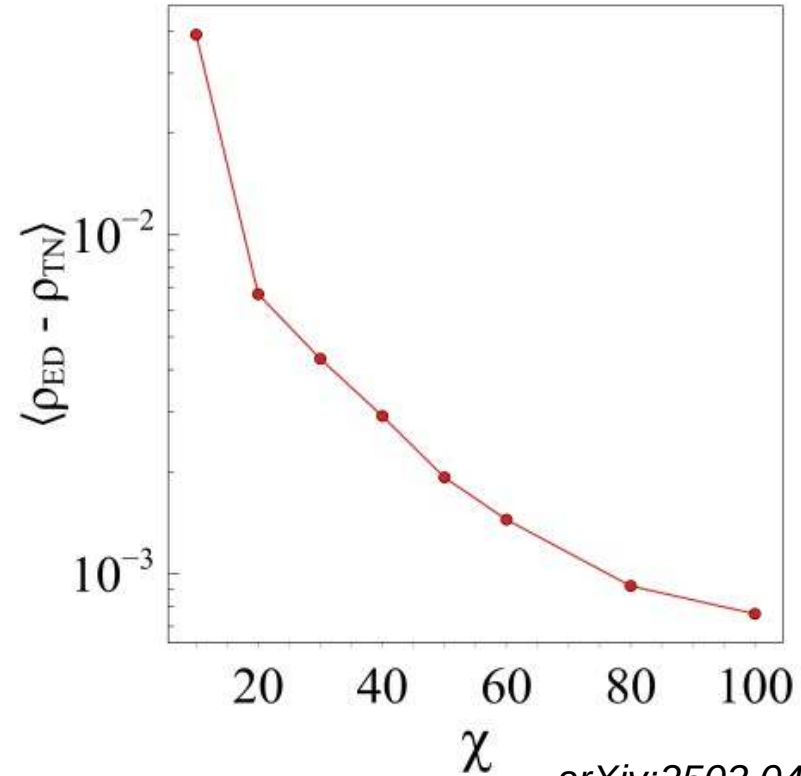


Computational performance of tight binding tensor networks

Time VS system size



Accuracy VS bond dimension



Topological invariants in real-space

The density matrix of a super-moire system can be expressed as a tensor network

$$\hat{\mathcal{P}} = \int_{-\infty}^{\varepsilon_F} \delta(\omega - \hat{H}) d\omega = \sum \Xi_{s_1, s'_1}^{(1)} \Xi_{s_2, s'_2}^{(2)} \cdots \Xi_{s_L, s'_L}^{(L)} |s\rangle \langle s'|$$

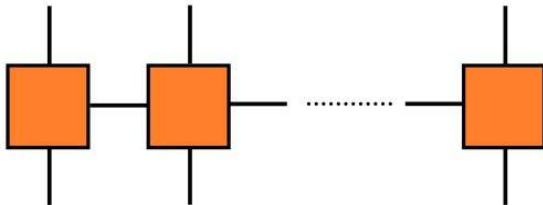
With a kernel polynomial tensor network algorithm

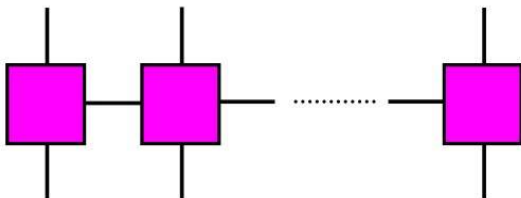
$$\hat{\mathcal{P}} = \sum_n T_n(\hat{\mathcal{H}}) \int_{-\infty}^{\varepsilon_F} d\omega \frac{T_n(\omega)}{\sqrt{1 - \omega^2}},$$

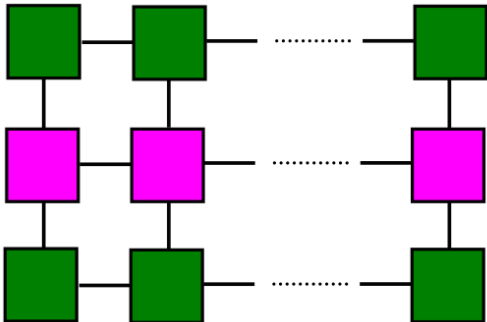
$$T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x)$$

$$T_0 = 1 \text{ and } T_1(x) = x$$

Computing Chern numbers with tensor networks

Density matrix as tensor network $\hat{P} = \int_{-\infty}^{\varepsilon_F} \delta(\omega - \hat{H}) d\omega =$ 

Topological marker as tensor network $\hat{\Gamma} = \hat{Q}\hat{X}\hat{P}\hat{Y}\hat{Q} - \hat{P}\hat{X}\hat{Q}\hat{Y}\hat{P} =$ 

Chern number from tensor network contraction $C_\alpha = 2\pi i \langle \alpha | \hat{\Gamma} | \alpha \rangle =$ 

Tensor network topological marker

Real-space Chern number (Chern marker)

$$C_{\alpha} = 2\pi i \langle \alpha | \hat{Q} \hat{X} \hat{P} \hat{Y} \hat{Q} - \hat{P} \hat{X} \hat{Q} \hat{Y} \hat{P} | \alpha \rangle$$

Tensor-network Chern marker

$$\hat{C}_{\alpha} = 2\pi i \left(\begin{array}{c} \hat{Q} \\ \hat{y}_{\alpha}^{\Lambda} \\ \hat{P} \\ \hat{x}_{\alpha}^{\Lambda} \\ \hat{Q} \end{array} \begin{array}{c} \text{---} \end{array} \begin{array}{c} \hat{P} \\ \hat{y}_{\alpha}^{\Lambda} \\ \hat{Q} \\ \hat{x}_{\alpha}^{\Lambda} \\ \hat{P} \end{array} \right)$$

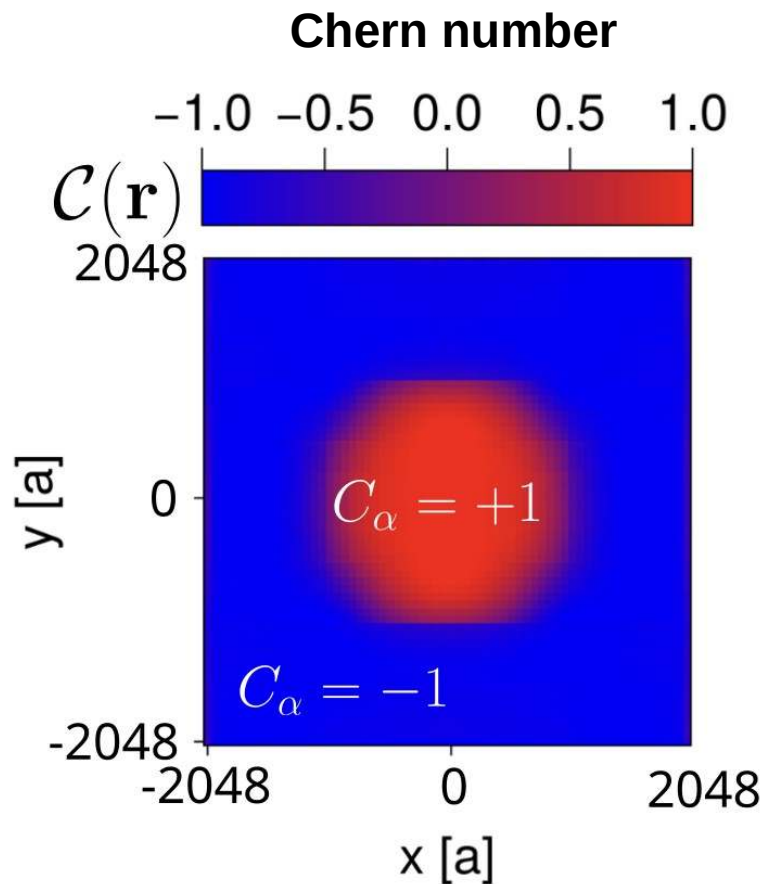
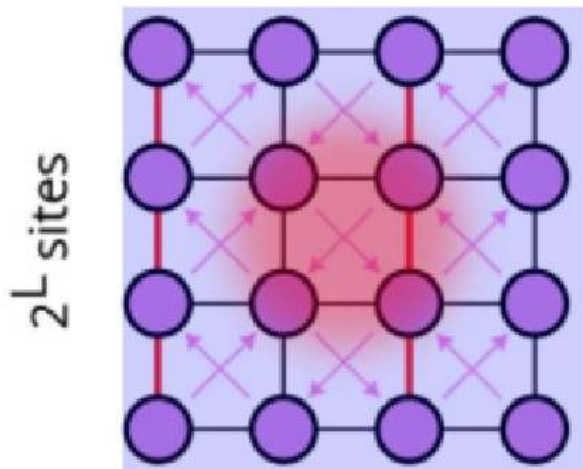
Topological domain with tensor networks

arXiv:2506.05230 (2025)

Topological marker

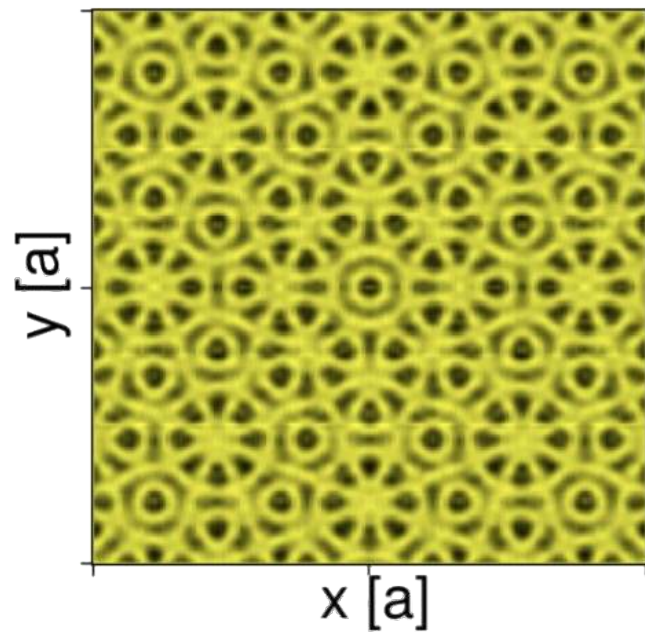
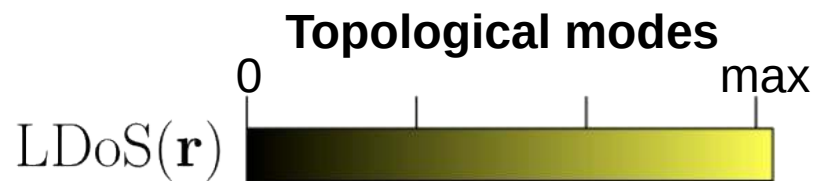
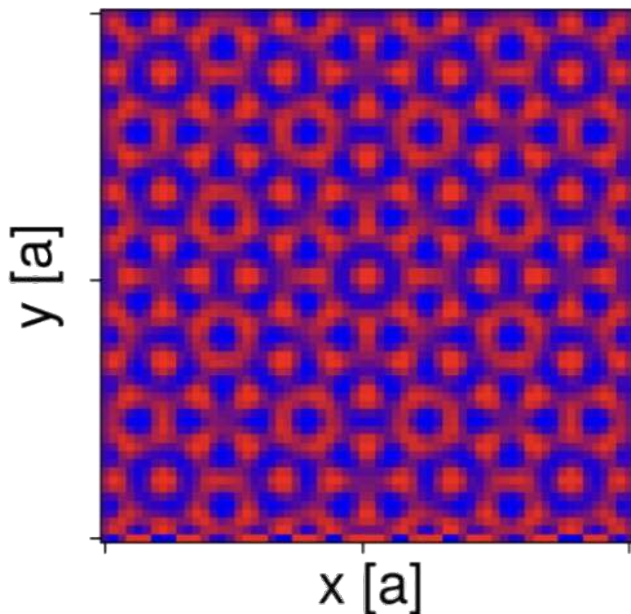
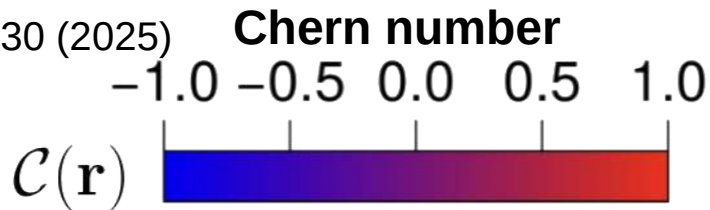
$$C_{\alpha} = 2\pi i \langle \alpha | \hat{Q} \hat{X} \hat{P} \hat{Y} \hat{Q} - \hat{P} \hat{X} \hat{Q} \hat{Y} \hat{P} | \alpha \rangle$$

**In a spatially modulated
topological Hamiltonian**



Super-moire topological matter with tensor networks

arXiv:2506.05230 (2025)



Tensor networks allow computing topology in exceptionally large super-moire systems

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

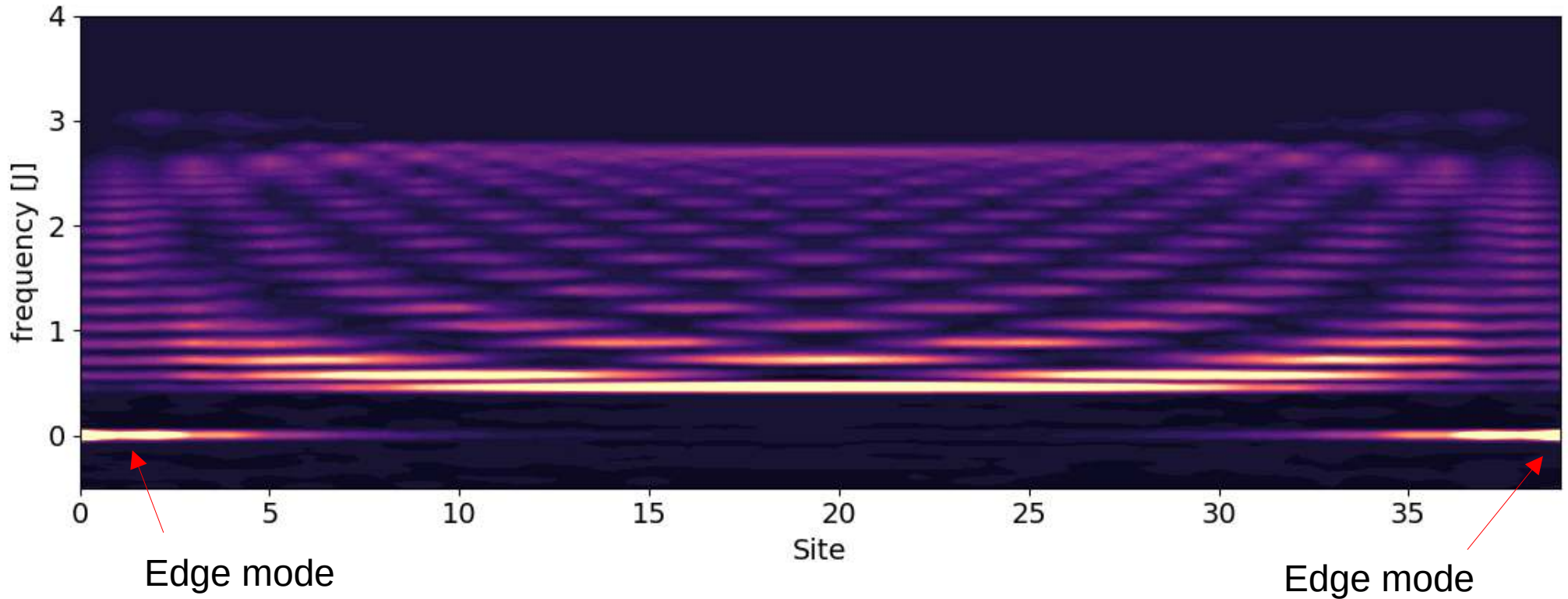
```
from dmrgpy import spinchain
spins = ["S=1" for i in range(40)] # S=1 chain
sc = spinchain.Spin_Chain(spins) # create spin chain object
h = 0 # initialize Hamiltonian
for i in range(len(spins)-1):
    h = h + sc.Sx[i]*sc.Sx[i+1]
    h = h + sc.Sy[i]*sc.Sy[i+1]
    h = h + sc.Sz[i]*sc.Sz[i+1]
sc.set_hamiltonian(h)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

dmrgpy

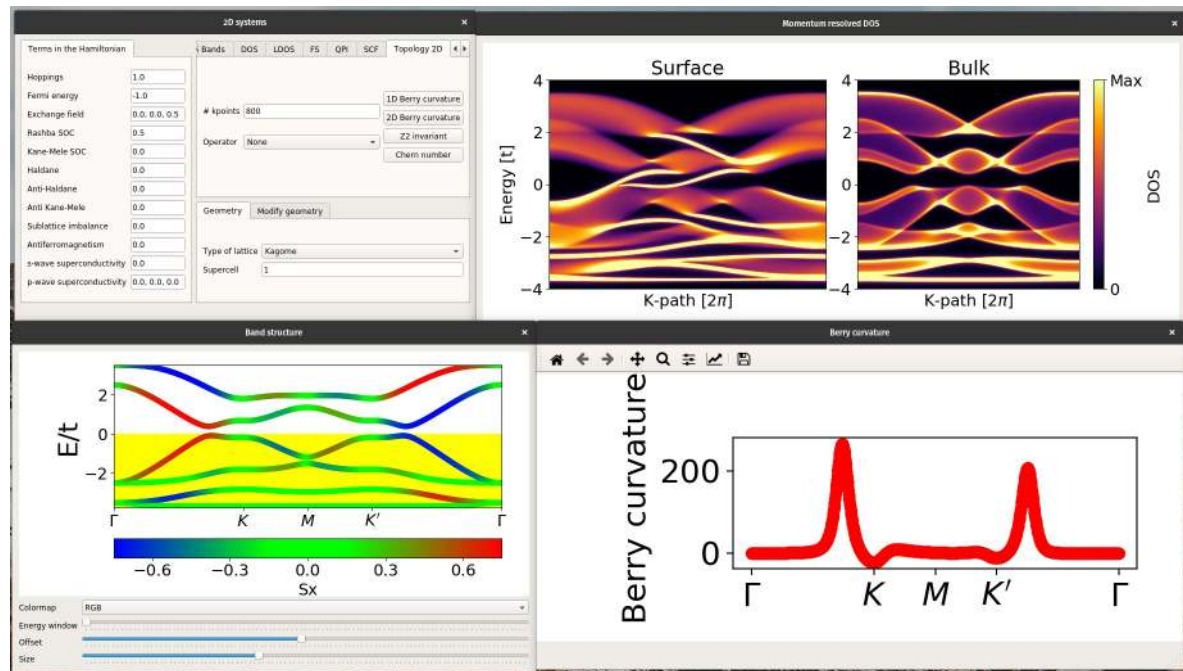
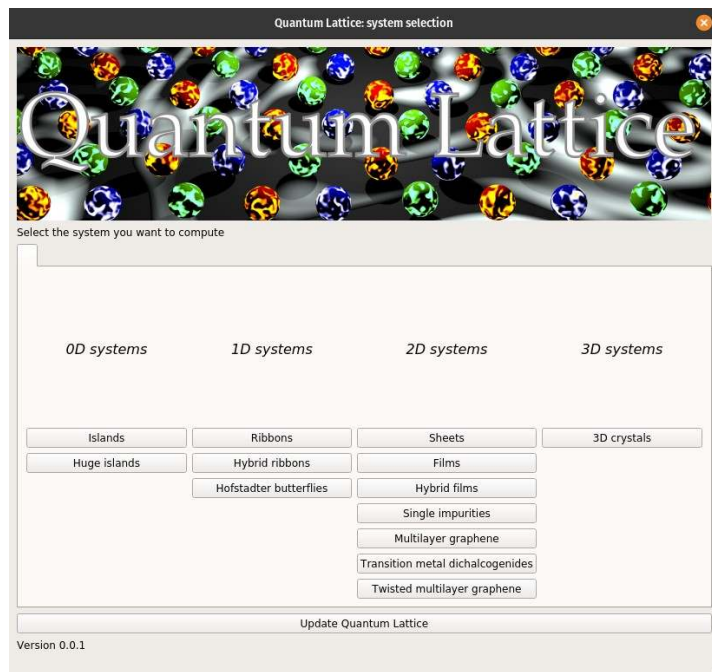
<https://github.com/joselado/dmrgpy>

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

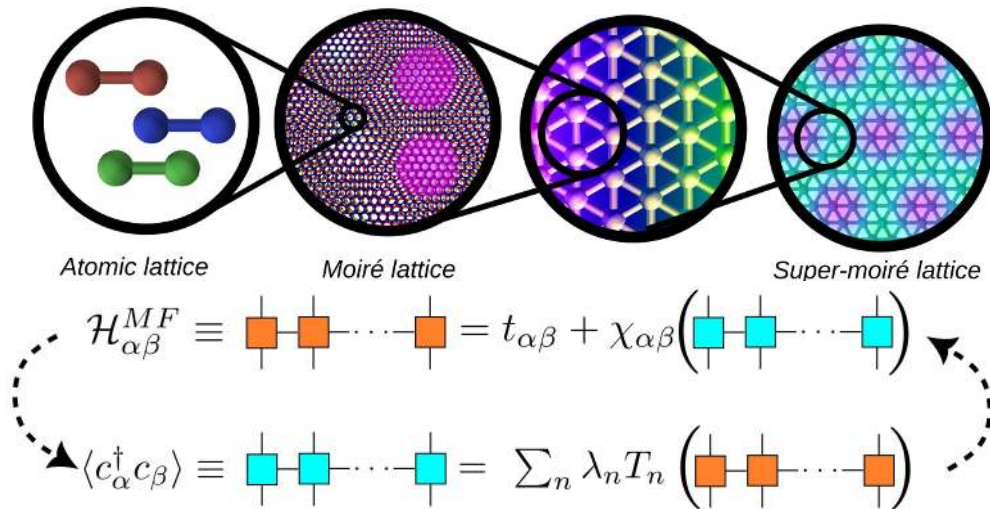


Quantum Lattice: open source interactive interface for tight binding modeling

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

Take home

Tensor network machine learning allows solving exponentially large electronic structure problems, reaching the regime required for super-moire materials



2D Materials 12 (1), 015018 (2025)
arXiv:2503.04373 (2025)
arXiv:2506.05230 (2025)

Funding from



Finnish Quantum Flagship



JANE AND AATOS
ERKKO FOUNDATION

