Solving billion-size super-moire quantum materials with quantum-inspired tensor network algorithms

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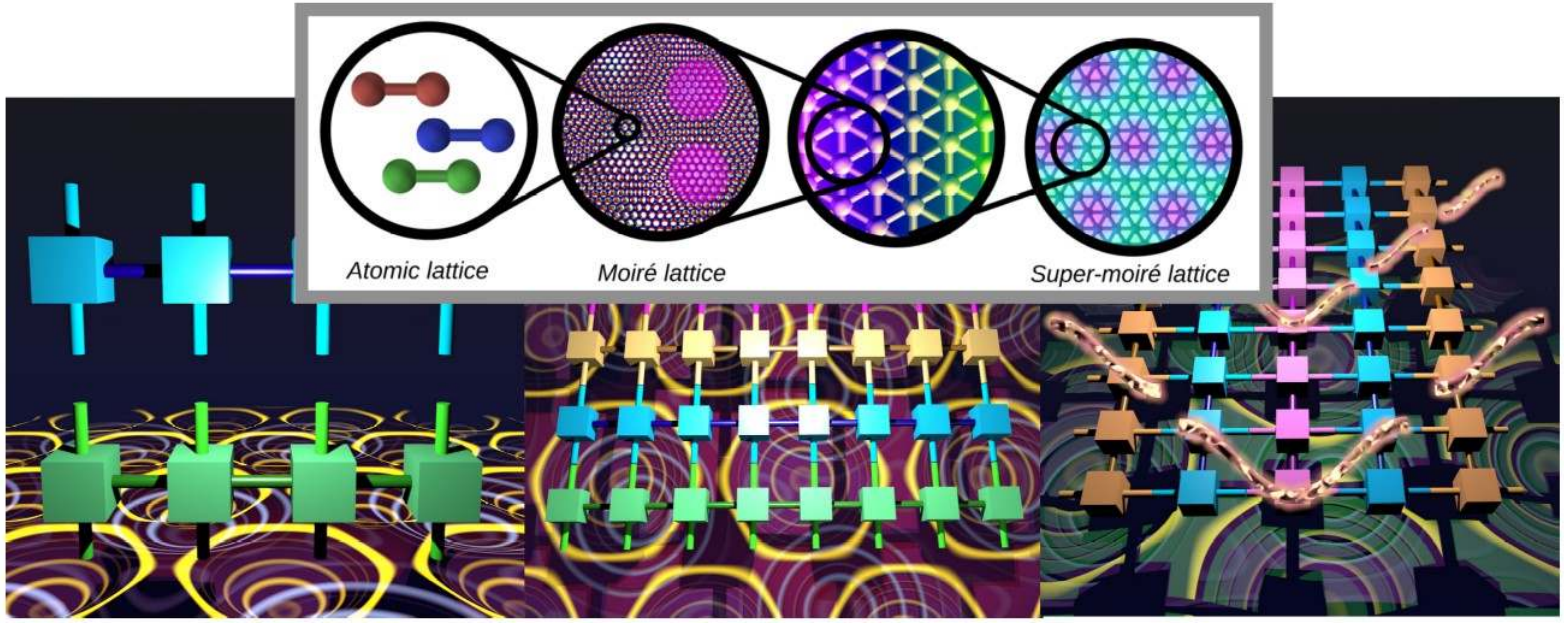


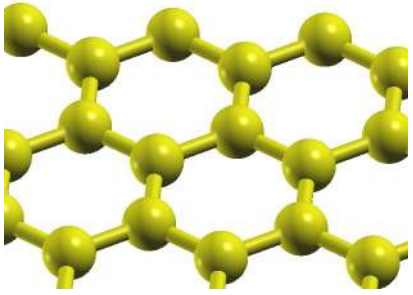
Phys. Rev. Research 7, 043288 (2025) *Phys. Rev. Lett. 136, 156601 (2026)* *arXiv:2512.18397 (2025)*

2D Day: Experimental and Theoretical Research on 2D Quantum Materials and Related Systems
Aalto University, May 19th 2026

A rich family of electronic orders in 2D materials

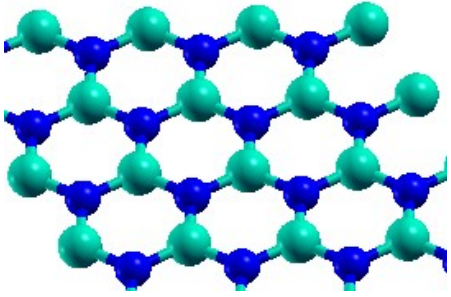
Semimetal

Graphene



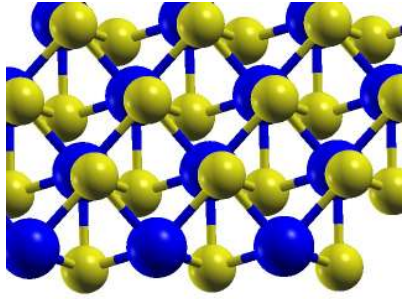
Insulator

BN



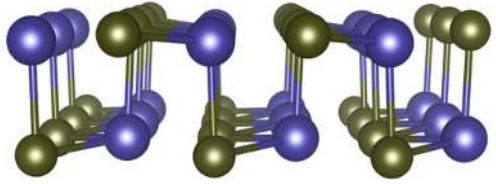
Superconductor

$NbSe_2$



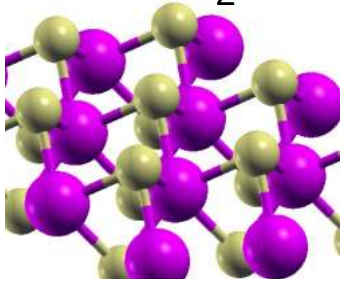
Ferroelectric

SnTe



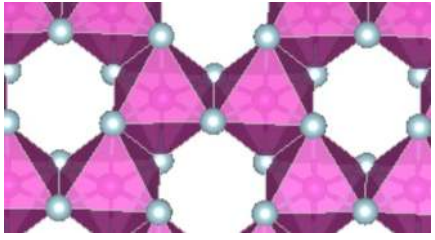
Semiconductor

WS_2



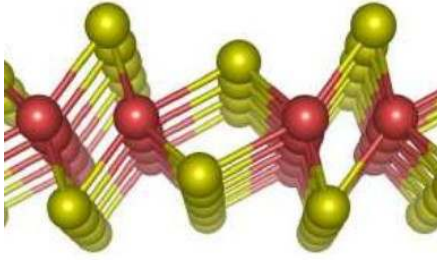
Ferromagnet

CrI_3



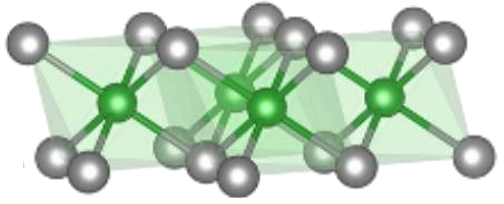
Quantum spin Hall insulator

WTe_2



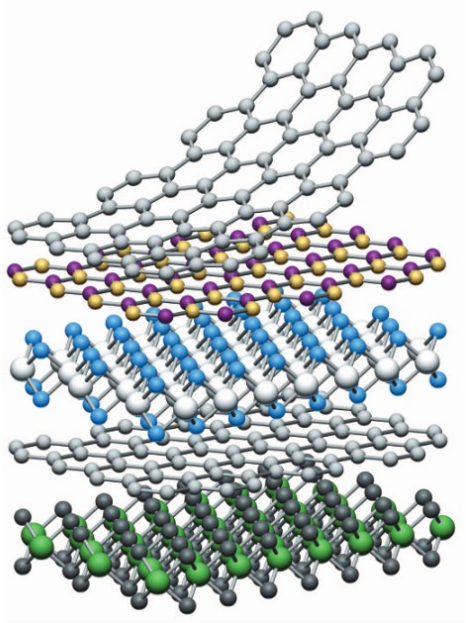
Multiferroic

NiI_2



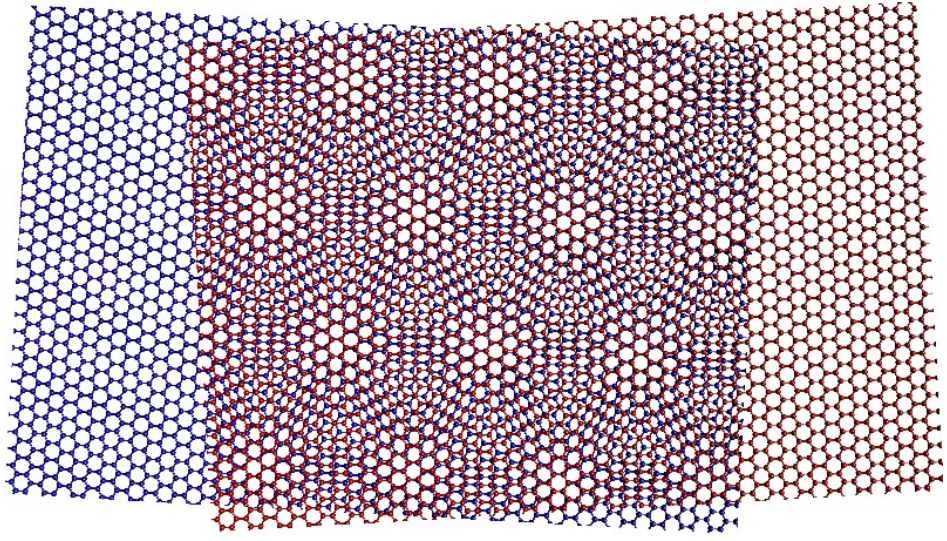
The flexibility of two-dimensional materials

They can be stacked



Nature 499, 419–425 (2013)

They can be rotated

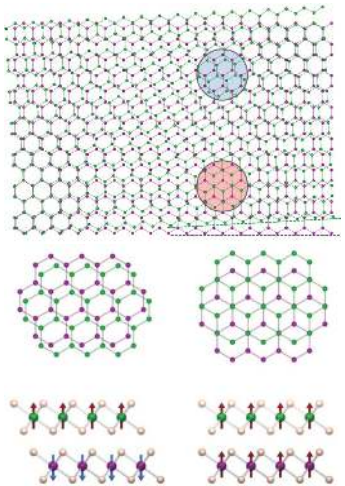


Science 361, 6403, 690-693 (2018)

These are unique features of two-dimensional materials

Artificial quantum matter in moire van der Waals heterostructures

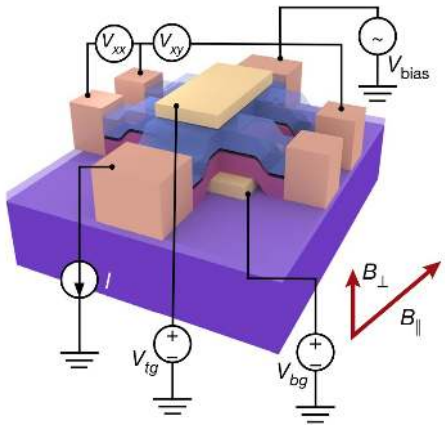
Unconventional magnets



Twisted $CrBr_3$

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

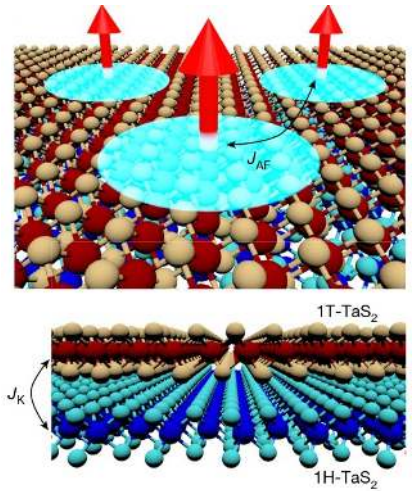
Unconventional superconductors



Twisted trilayer graphene

Nature 595, 526–531 (2021)

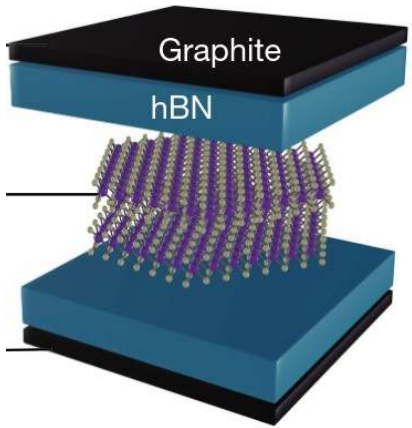
Heavy-fermion quantum materials



1H-1T TaS_2

Nature 599, 582–586 (2021)

Fractional topological matter

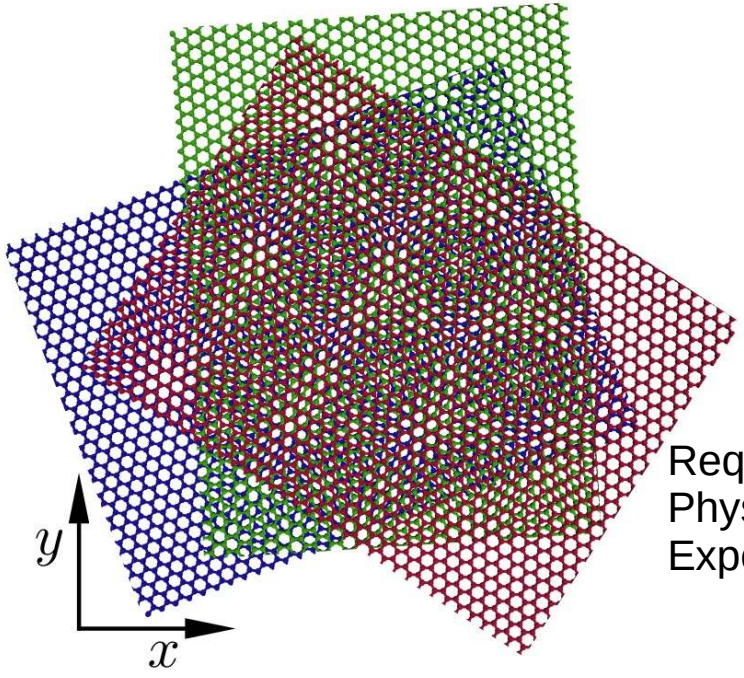


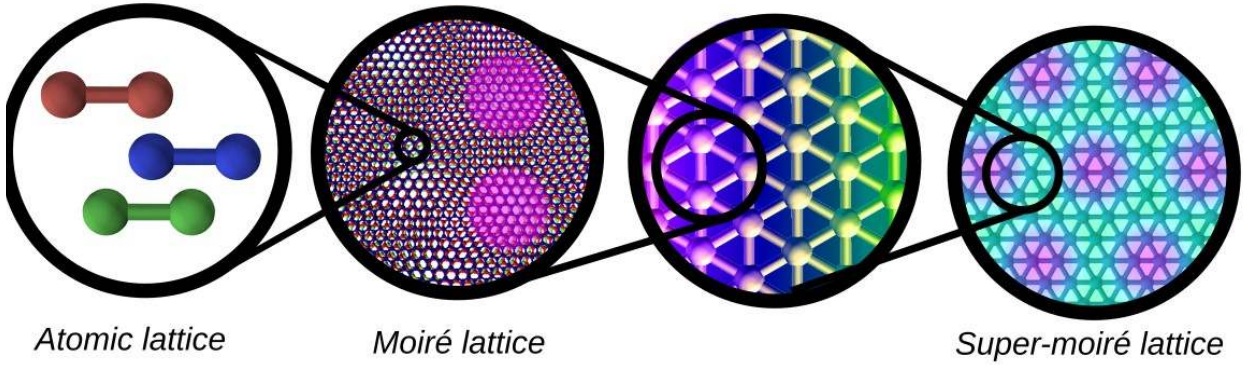
Twisted $MoTe_2$

Nature 622, 63–68 (2023)

Super-moire materials

Moire-of-moire materials



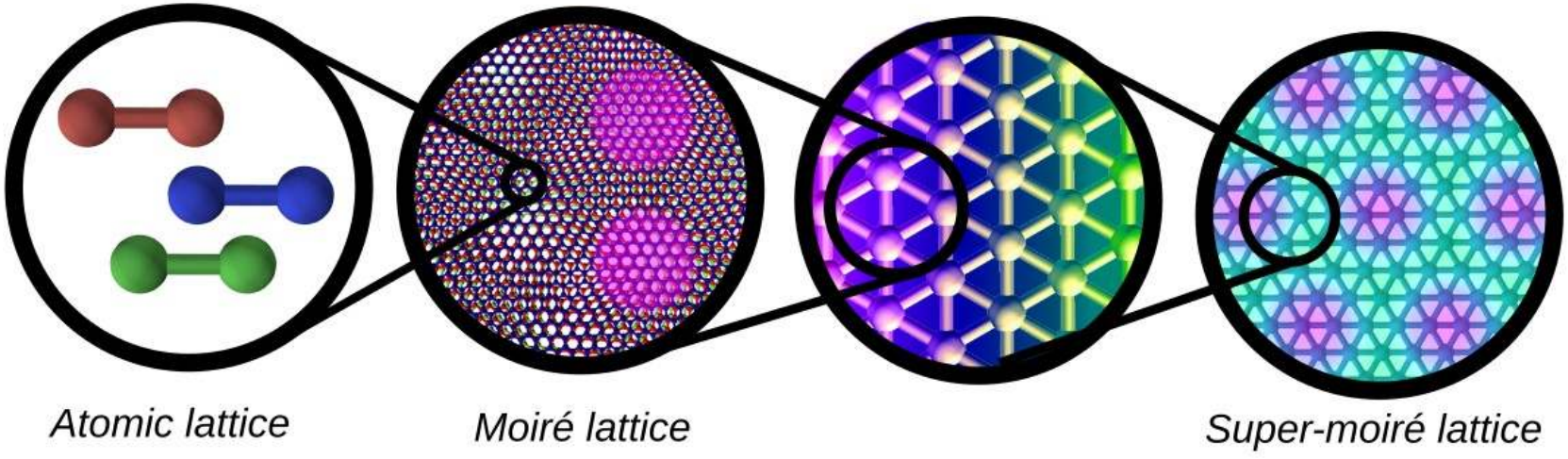


Requires computing up to a billion sites (10^9)
Physics at several length scales (atomic, moire, and super-moire)
Experiments showing correlations and unconventional superconductivity

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)



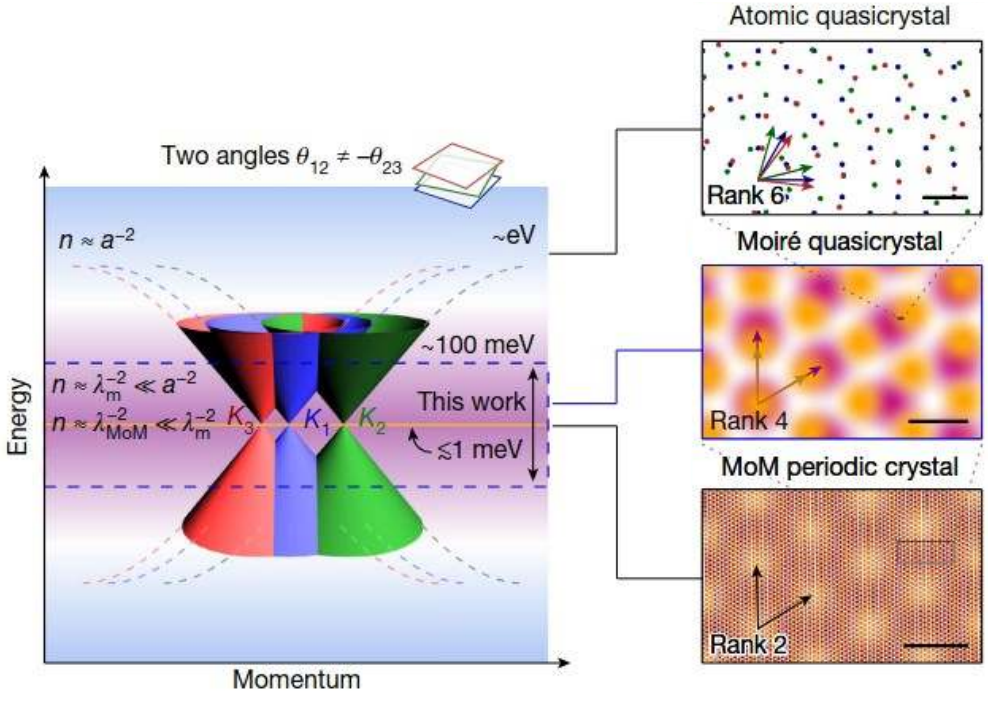
Moire systems **N=10^5 sites**, calculations taking around 1 minute
Computational cost grows as **N** (best case) or **N^3** (worst case)
Super-moire **N=10^9 sites**, calculations taking 10 days – 1000000 years

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

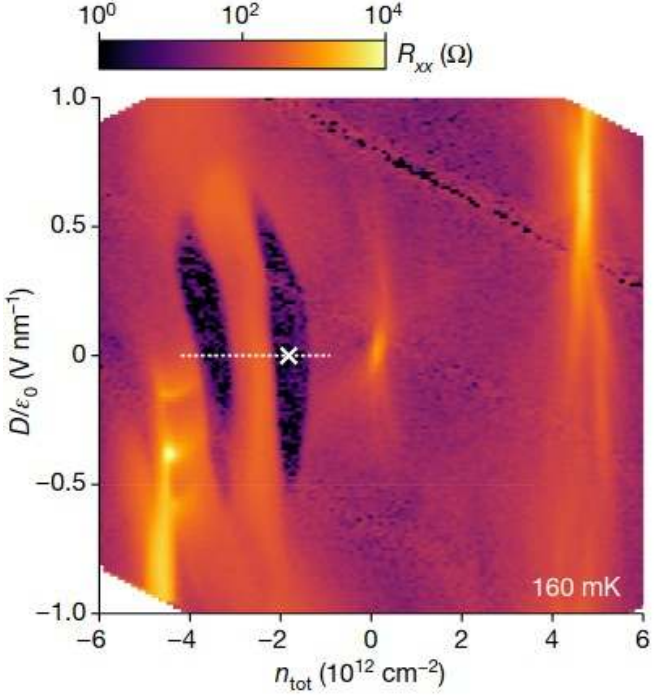
(even going beyond usual memory limitations of conventional methods)

Super-moire materials, experimentally

Moire quasicrystal in twisted trilayer graphene



Coexisting correlations and superconductivity



Nature 620, 762–767 (2023)

Behind the scenes

Yitao Sun

Tiago Antão

Anouar Moustaj

Marcel Niedermeier

Adolfo Fumega

Self-consistent tensor network method for correlated super-moire matter beyond one billion sites, Y. Sun, M. Niedermeier, T. V. C. Antão, A. O. Fumega, J. L. Lado, **Phys. Rev. Research 7, 043288 (2025)**

Tensor network method for real-space topology in quasicrystal Chern mosaics, T. V. C. Antão, Y. Sun, A. O. Fumega, J. L. Lado, **Phys. Rev. Lett. 136, 156601 (2026)**

Momentum-resolved spectral functions of super-moiré systems using tensor networks, A. Moustaj, Y. Sun, T. V. C. Antão, J. L. Lado, **arXiv:2512.18397 (2025)**

Encoding an exponentially large quantum many-body space with tensor networks

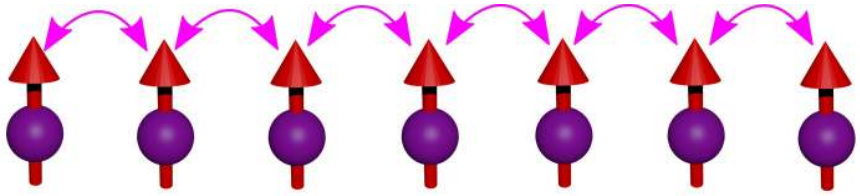
The problem of dimensionality

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

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

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

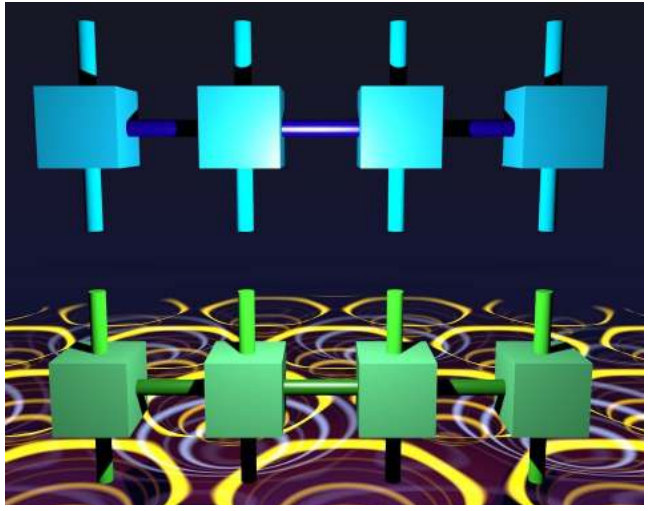
Is there an efficient way of storing so many coefficients?

Dealing with very large spaces with tensor networks

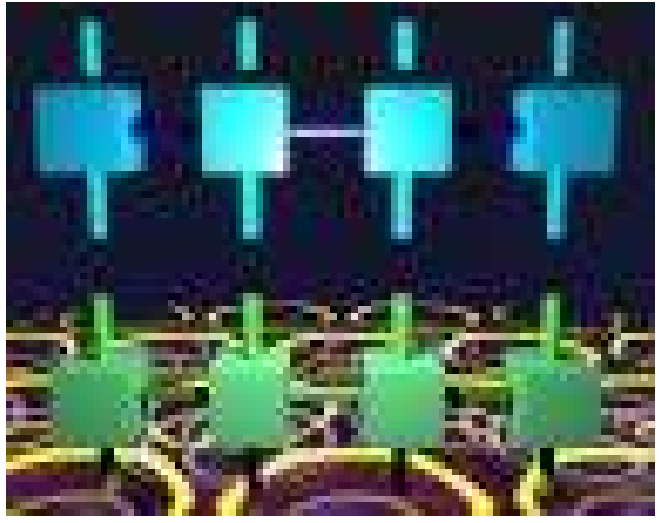
A many-body wavefunction a is a very high dimensional object (2^L coefficients)

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

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

Tensor networks allow parametrizing many-body wavefunctions as

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

$L\chi^2$ parameters

Full wavefunction  *Matrix product state*

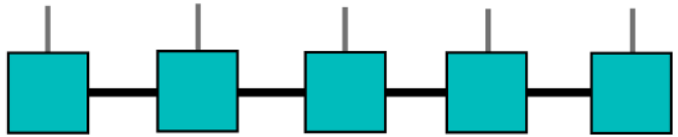
Tensor networks allow to drastically reduce the memory required to store a many-body state

Annals of Physics 326, 96 (2011)

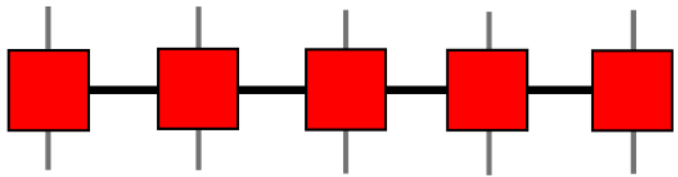
Exponentially large algebra with tensor networks

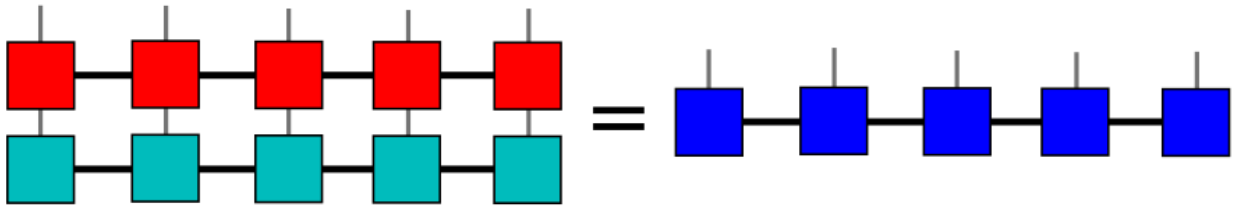
Tensor network allow to (approximately) operate in exponentially large vector spaces

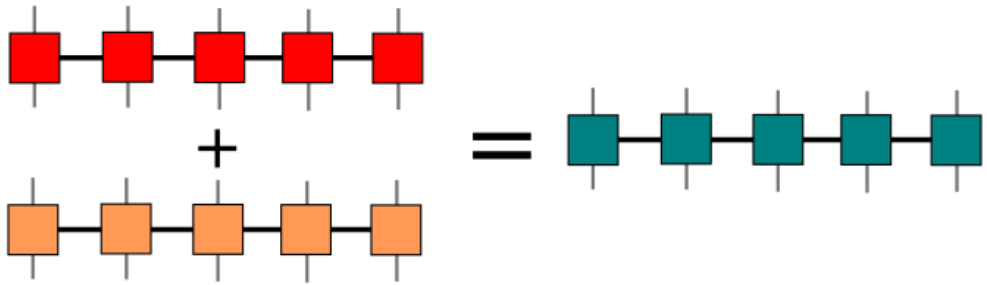
vector

$|\Psi\rangle \equiv$ 

matrix

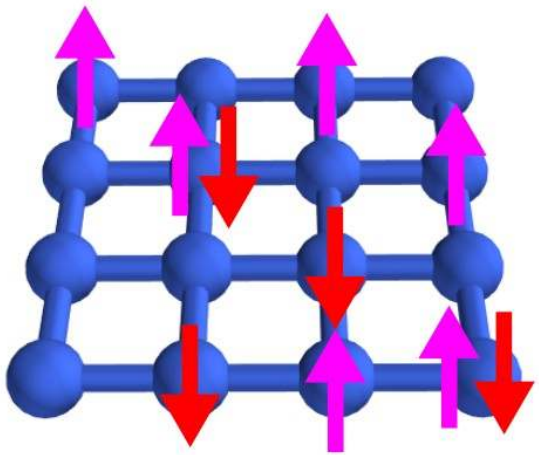
$\hat{A} \equiv$ 

$|\Psi_2\rangle = \hat{A}|\Psi_1\rangle \equiv$ 

$\hat{A}_3 = \hat{A}_1 + \hat{A}_2 \equiv$ 

Some paradigmatic problems solved with matrix product states

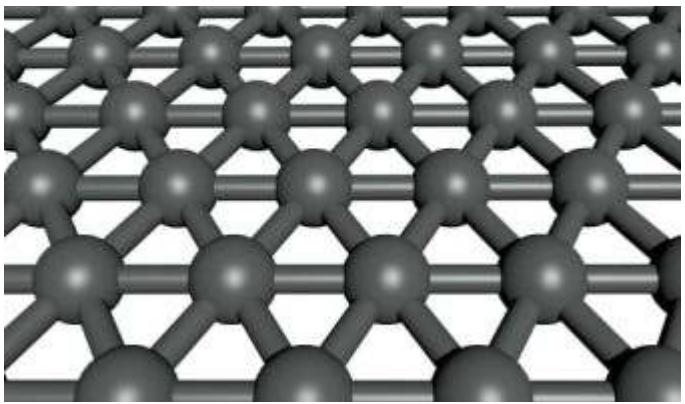
Solving the 2D Hubbard model at finite doping



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

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

Solving the 2D Heisenberg model in frustrated lattices

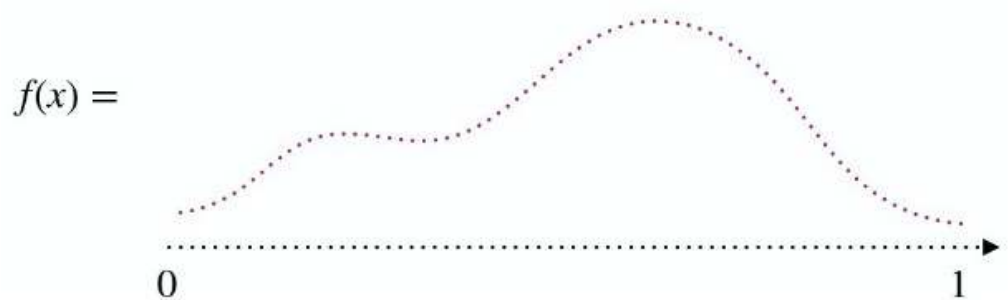


$$\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

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

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

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

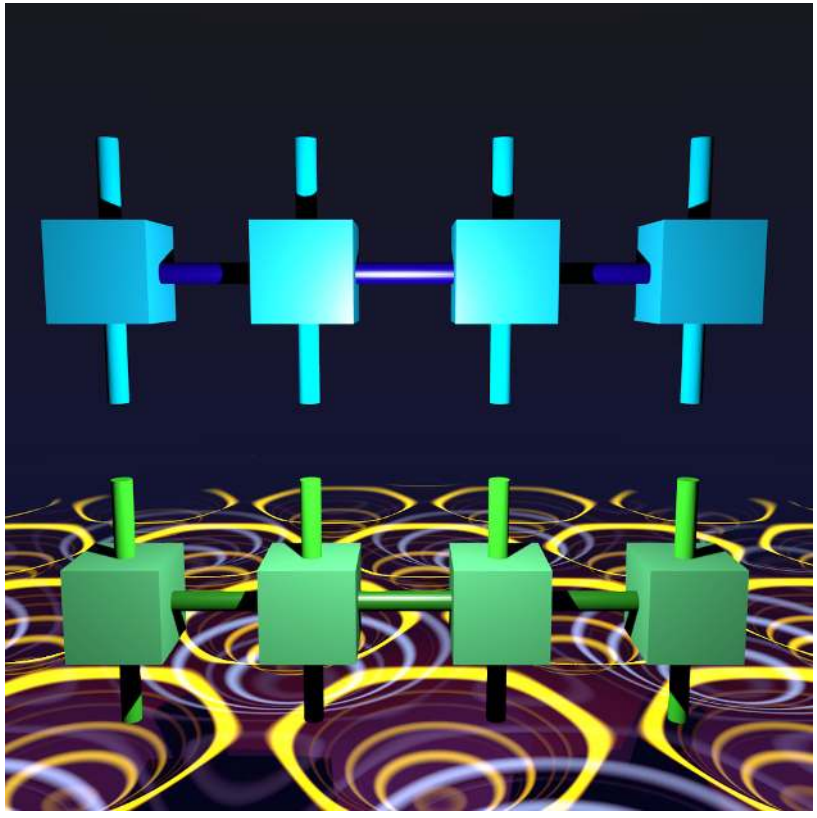
$$x = \sum_n 2^{-n} s_n \qquad f(x) = c_{s_1,s_2,\ldots,s_L} \qquad s_n = 0, 1$$

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

Quantum-inspired active learning algorithm

Phys. Rev. Lett. 132, 056501 (2024) SciPost Phys. 18, 104 (2025)

Tensor-networks for interacting super-moire materials



Phys. Rev. Research 7, 043288 (2025)

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Solving a correlated super-moire material with mean-field

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 networks for a super-moire tight binding problem

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

Many-body basis $|\uparrow\uparrow\uparrow\rangle$ $|\uparrow\uparrow\downarrow\rangle$ $|\uparrow\downarrow\uparrow\rangle$ $|\uparrow\downarrow\downarrow\rangle$ $|\downarrow\uparrow\uparrow\rangle$ $|\downarrow\uparrow\downarrow\rangle$ $|\downarrow\downarrow\uparrow\rangle$ $|\downarrow\downarrow\downarrow\rangle$

Single particle basis $c_1^\dagger|\Omega\rangle$ $c_2^\dagger|\Omega\rangle$ $c_3^\dagger|\Omega\rangle$ $c_4^\dagger|\Omega\rangle$ $c_5^\dagger|\Omega\rangle$ $c_6^\dagger|\Omega\rangle$ $c_7^\dagger|\Omega\rangle$ $c_8^\dagger|\Omega\rangle$

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

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

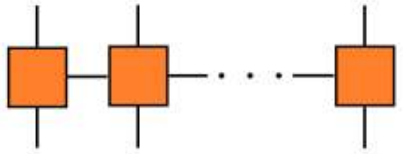
With quantics tensor-cross interpolation: ***<u>a quantum-inspired active learning algorithm</u>***

Phys. Rev. Lett. 132, 056501 (2024) SciPost Phys. 18, 104 (2025)

Self-consistent electronic interactions with tensor networks

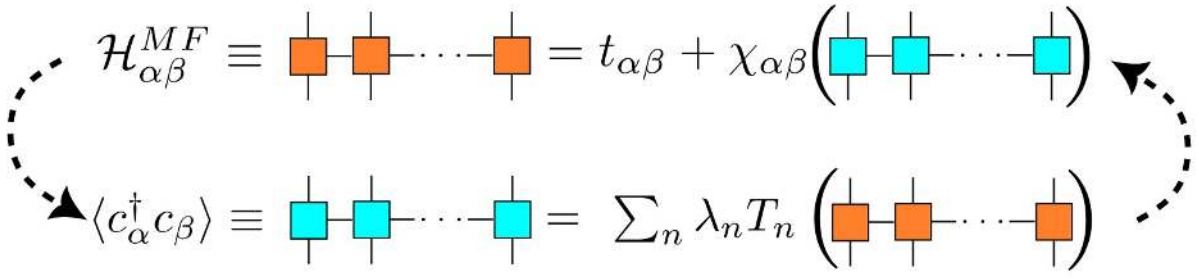
We represent the super-moire electronic Hamiltonian as a tensor-network

$$\mathcal{H}^{MF}_{\alpha\beta} \equiv \Gamma^{(1)}_{s_1,s_1'}\Gamma^{(2)}_{s_2,s_2'}\Gamma^{(3)}_{s_3,s_3'}...\Gamma^{(L)}_{s_L,s_L'}$$

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

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

Tensor Network SCF loop

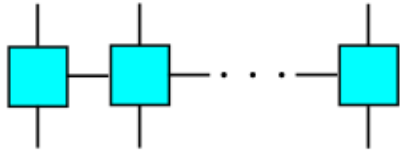


Phys. Rev. Research 7, 043288 (2025)

Kernel polynomial tensor network algorithm

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

$$\hat{\mathcal{P}} = \int_{-\infty}^{\varepsilon_F} \delta(\omega - \hat{H}) d\omega \equiv$$



With a kernel polynomial tensor network algorithm

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

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

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

Rev. Mod. Phys. 78, 275 (2006)
Phys. Rev. Research 7, 043288 (2025)

Spectral functions with tensor networks

Local spectral function of the mean-field Hamiltonian

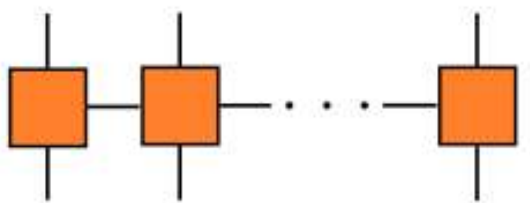
$$D(\omega,\alpha) = \langle\alpha| \left[\sum_n T_n(\mathcal{H}^{MF}) P_n(\omega)\right] |\alpha\rangle$$

With a tensor network Chebyshev algorithm

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

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

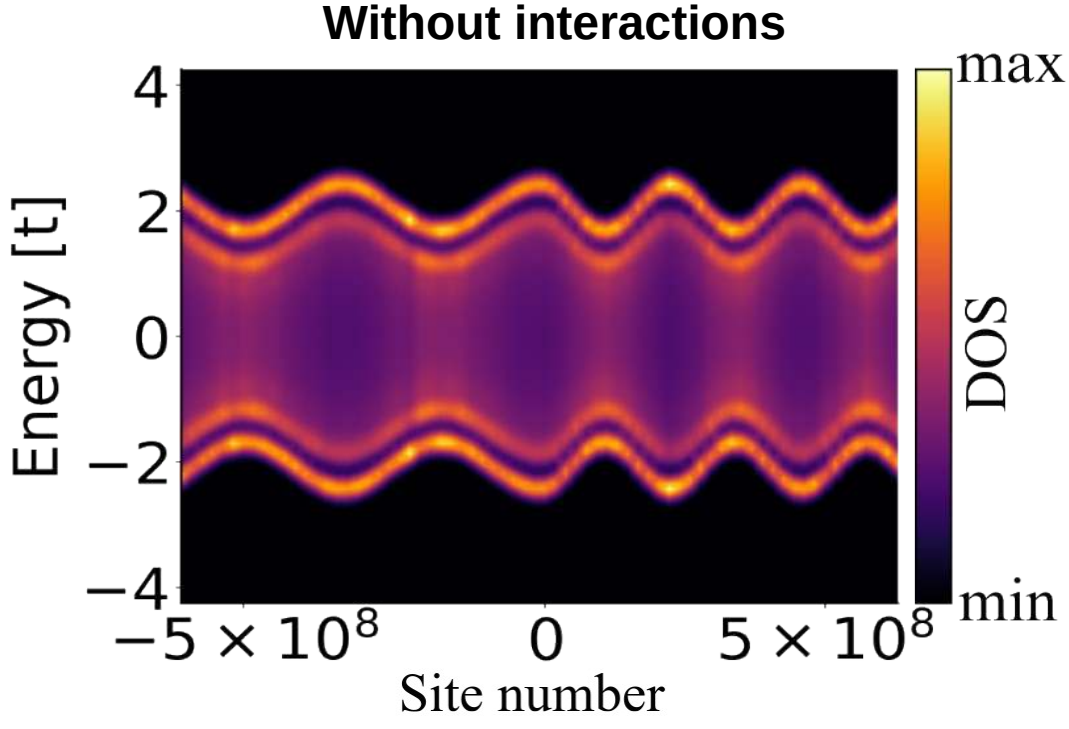
$$\mathcal{H}^{MF}_{\alpha\beta} \equiv$$

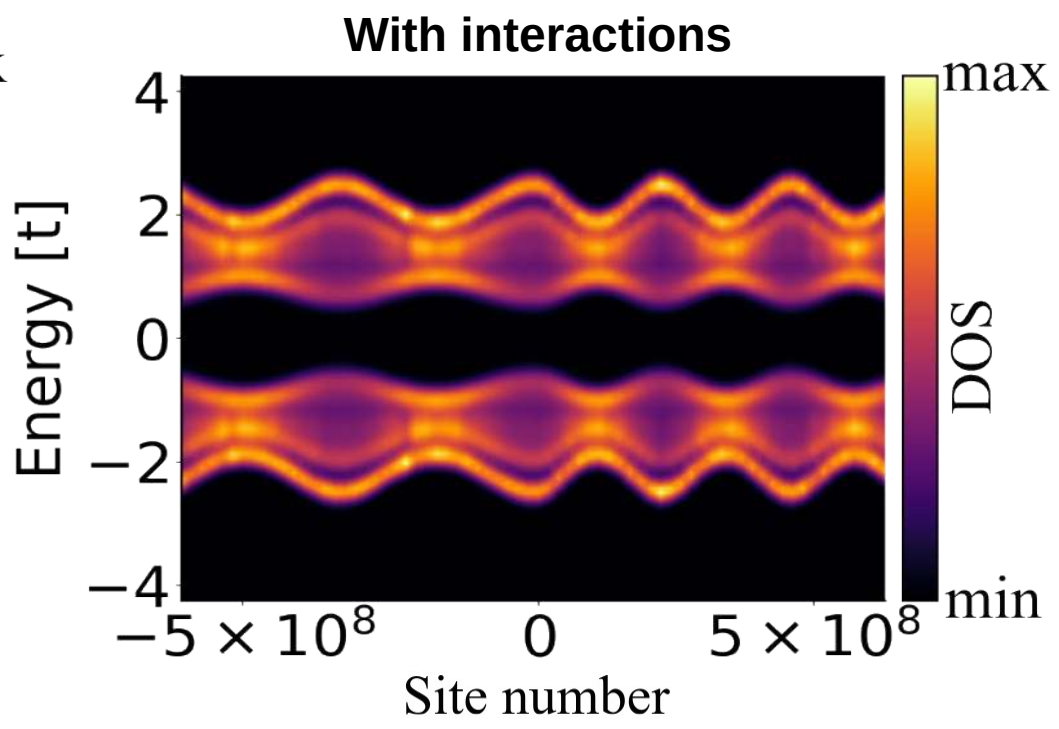


Rev. Mod. Phys. 78, 275 (2006)

Phys. Rev. Research 7, 043288 (2025)

Solving billion-size super-moire materials

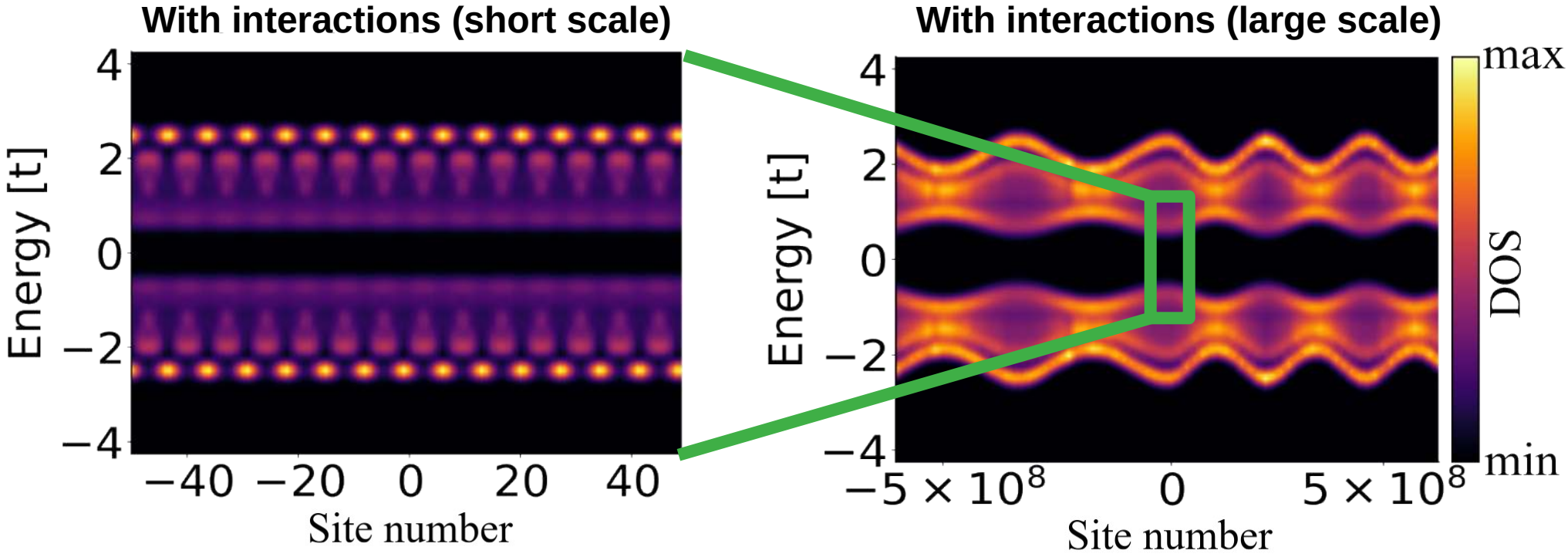




Tensor networks allow to solve selfconsistently a super-moire with one billion sites

Phys. Rev. Research 7, 043288 (2025)

Solving billion-size super-moire materials

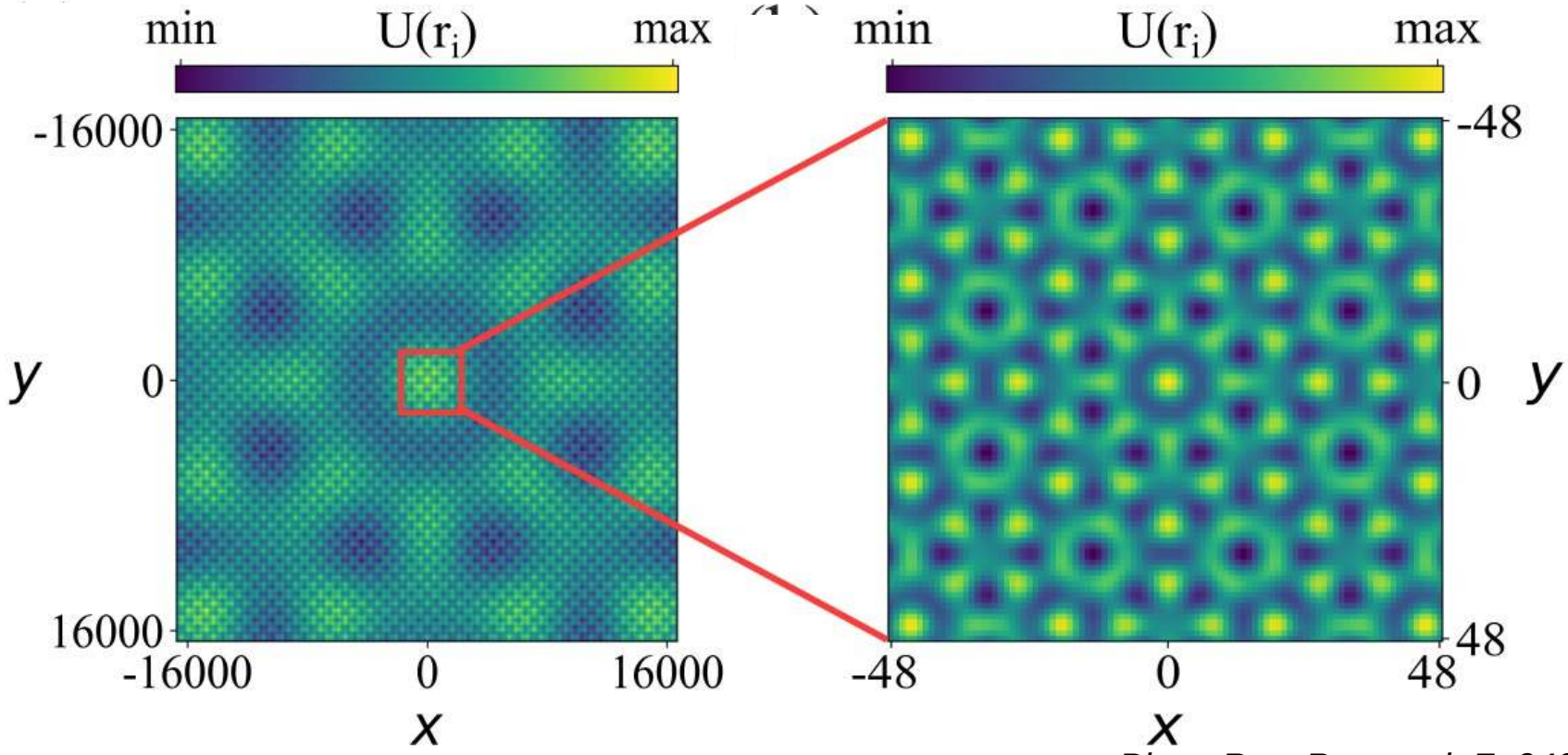


Tensor networks allow to solve selfconsistently a super-moire with one billion sites

Phys. Rev. Research 7, 043288 (2025)

Two-dimensional billion size interacting super-moire

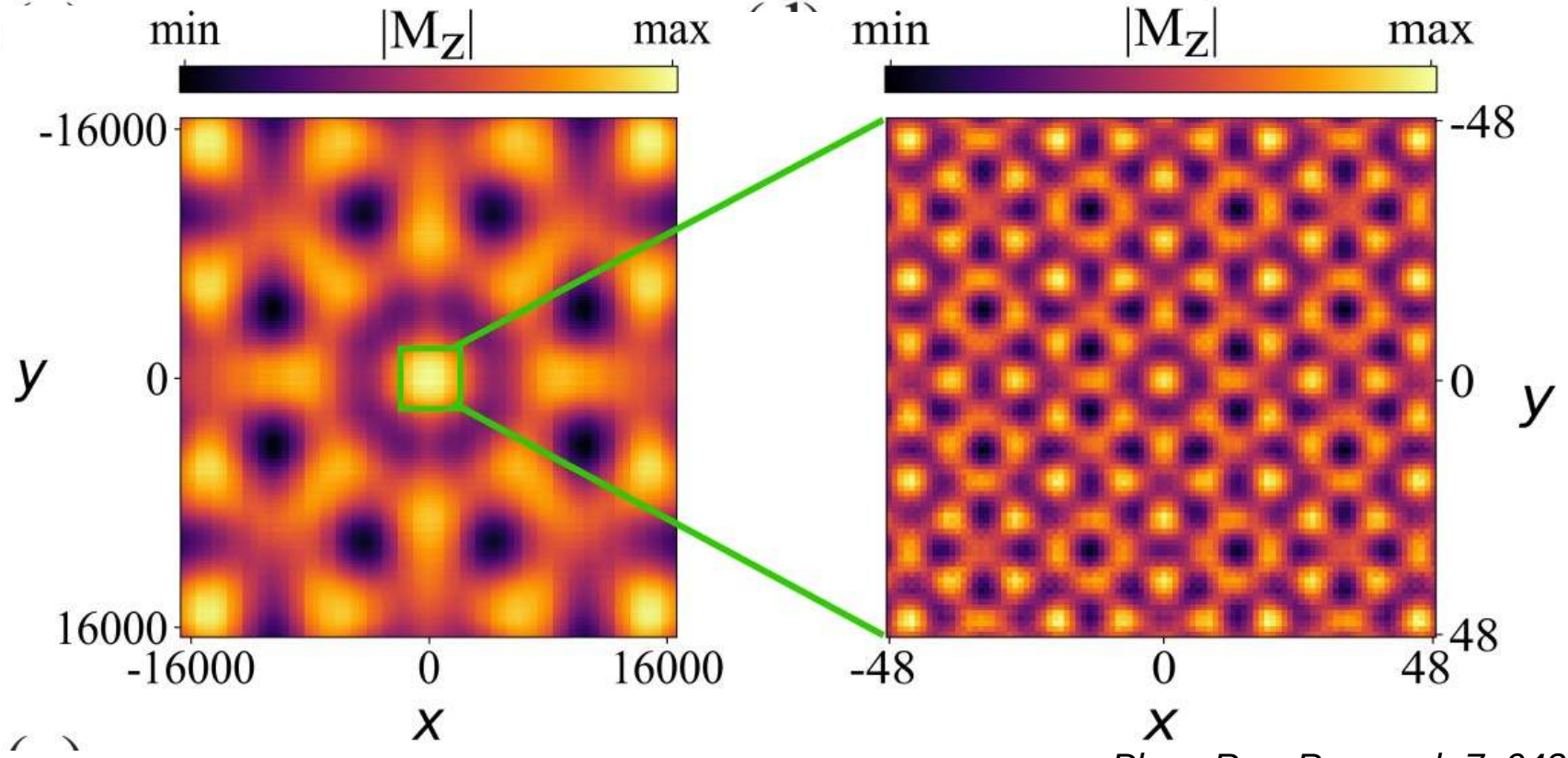
Modulation fo the Hamiltonian



Phys. Rev. Research 7, 043288 (2025)

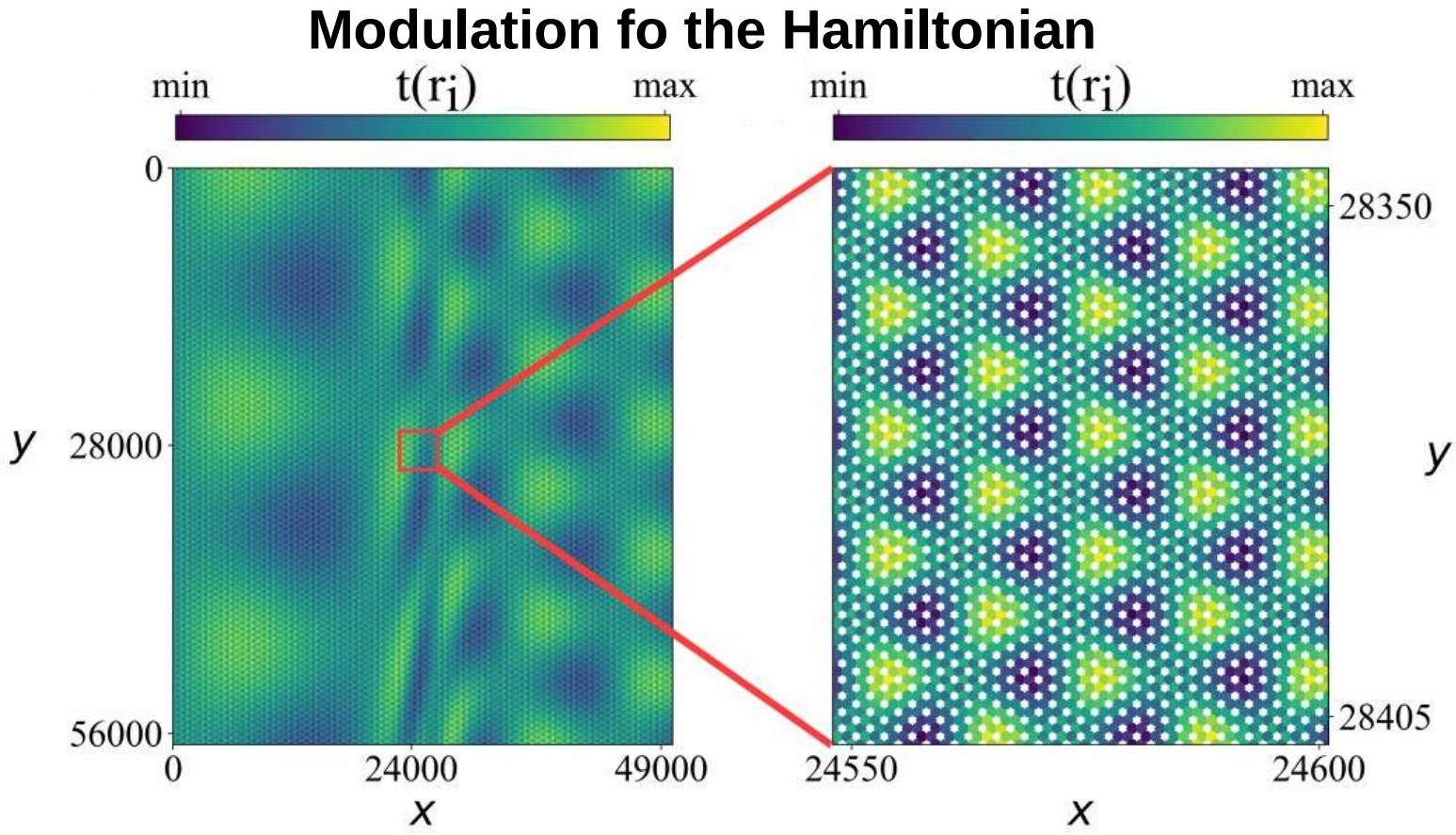
Two-dimensional billion size interacting super-moire

Selfconsistent symmetry broken order (magnetization)



Phys. Rev. Research 7, 043288 (2025)

Two-dimensional billion size interacting super-moire



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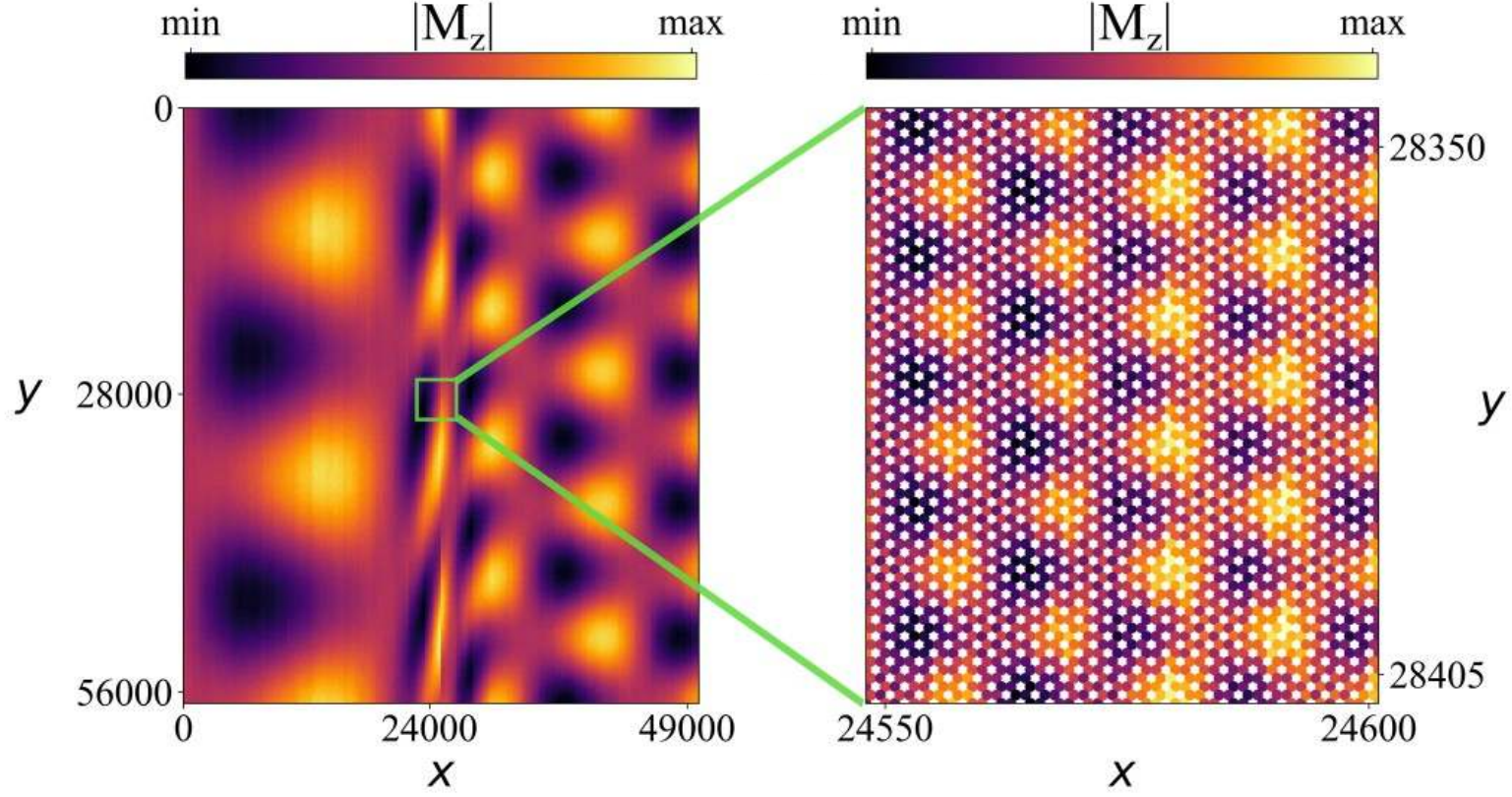
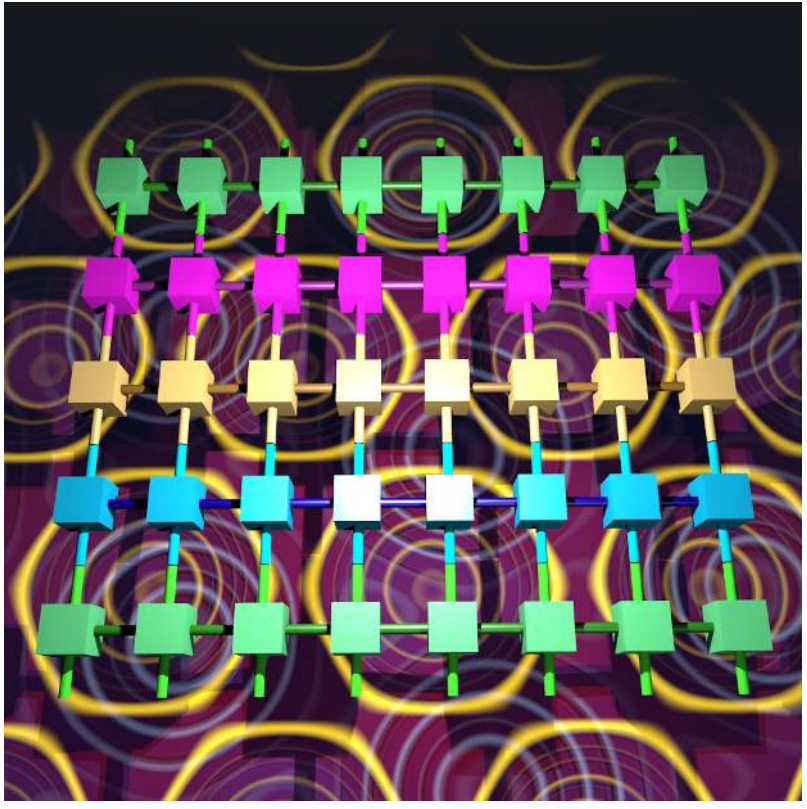


Tensor networks for topological super-moire materials



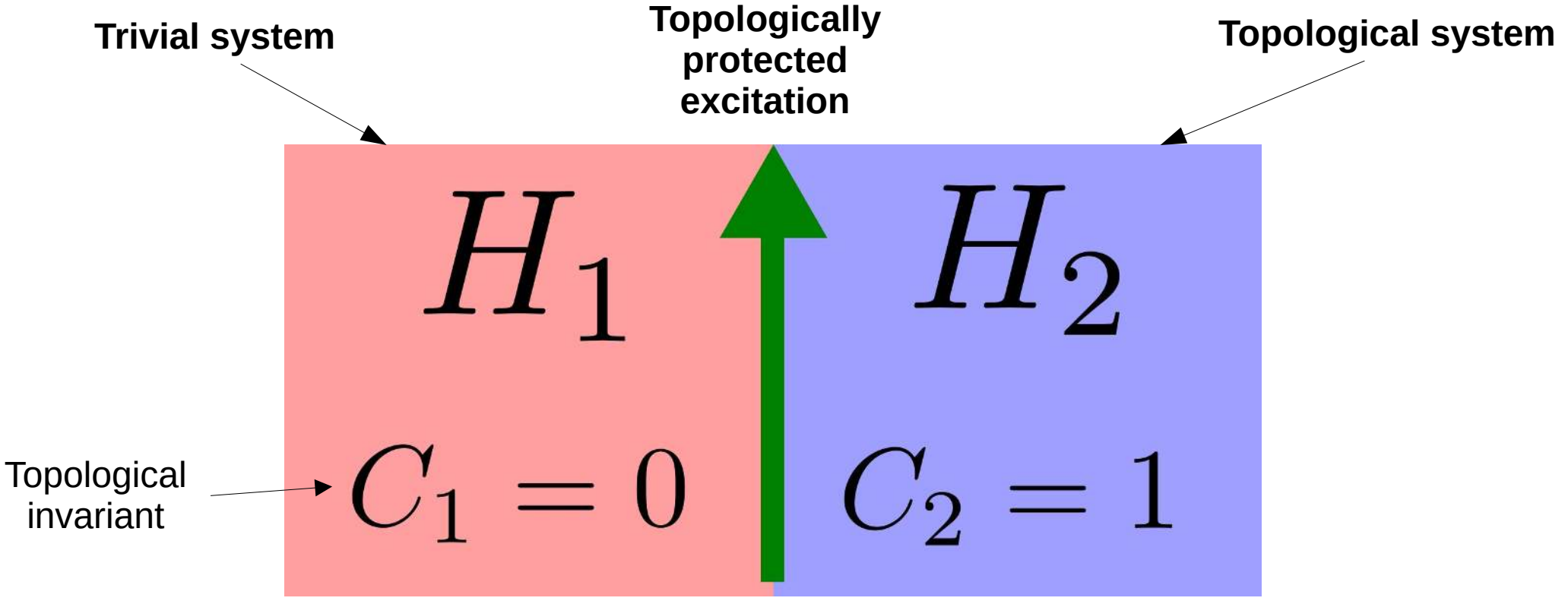
Yitao Sun

Tiago Antão

Adolfo Fumega

Phys. Rev. Lett. 136, 156601 (2026)

Topological states and edge modes



Topological excitations appear between topologically different systems

Real space topological invariants

Topological invariants are often defined in reciprocal space

$$C = \int_{BZ} \Omega d^2\mathbf{k}$$

$$\Omega_\alpha = \partial_{k_x} A_y^\alpha - \partial_{k_y} A_x^\alpha$$

$$A_\mu^\alpha = i\langle \partial_{k_\mu} \Psi_\alpha | \Psi_\alpha \rangle$$

Is it possible to define them in real space?

Real-space Chern number

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

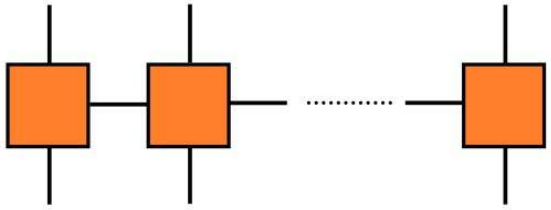
$$\hat{P} = \int_{-\infty}^{\epsilon_F} \delta(\omega - H) d\omega$$

$$\hat{Q} = 1 - \hat{P}$$

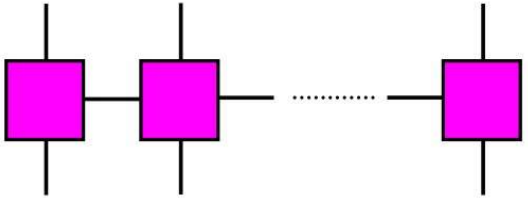
Phys. Rev. B 84, 241106R (2011)

Computing Chern numbers with tensor networks

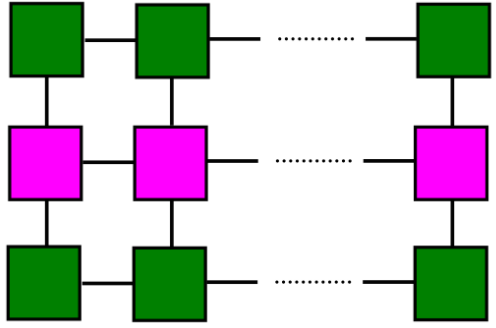
Density matrix as tensor network $\hat{P} = \int_{-\infty}^{\varepsilon_F} \delta(\omega - \hat{H}) d\omega =$



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 $C_\alpha = 2\pi i \langle \alpha | \hat{\Gamma} | \alpha \rangle =$



Phys. Rev. Lett. 136, 156601 (2026)

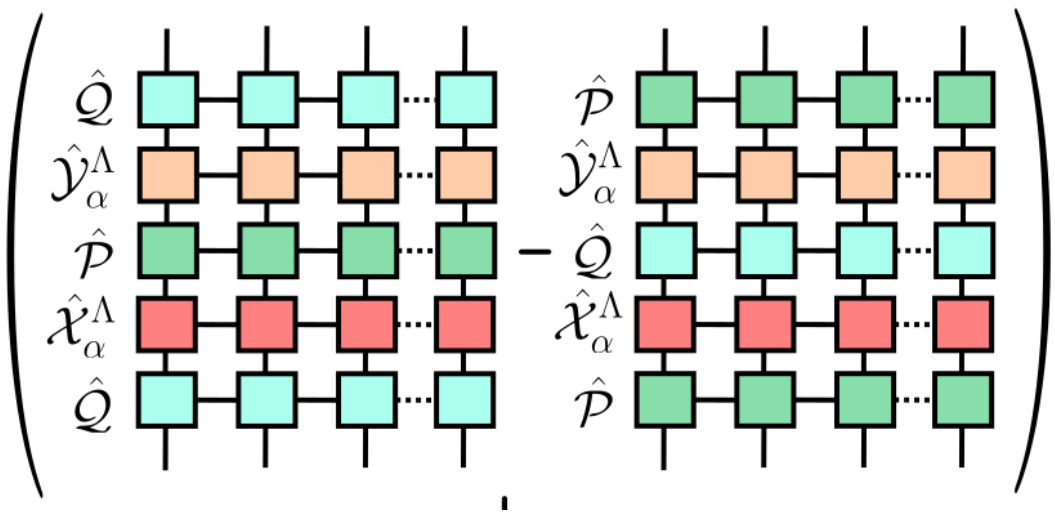
Tensor network topological marker

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

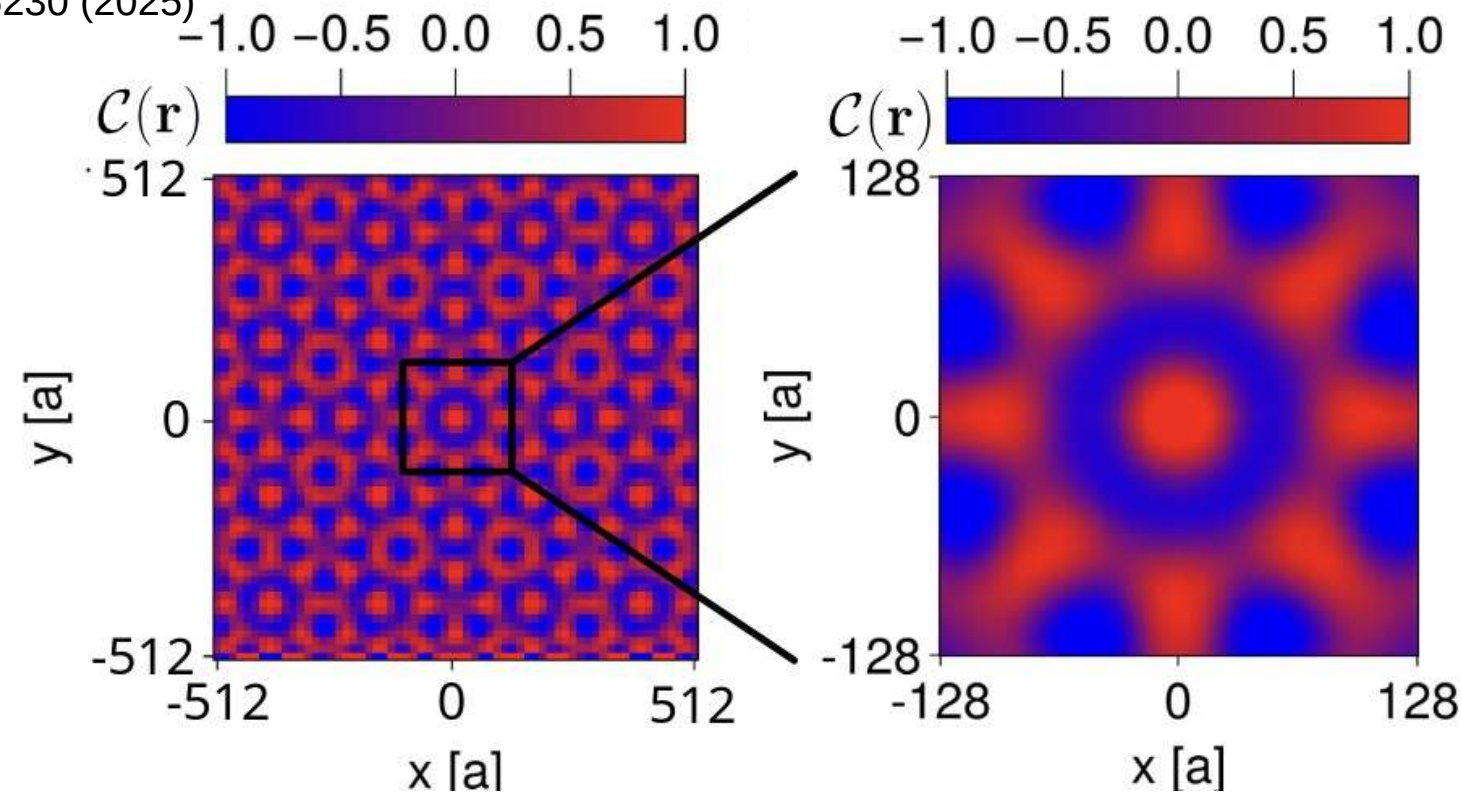
$$\hat{\mathcal{C}}_\alpha = 2\pi i$$



Phys. Rev. Lett. 136, 156601 (2026)

Chern mosaic in a 8-fold topological quasicrystal

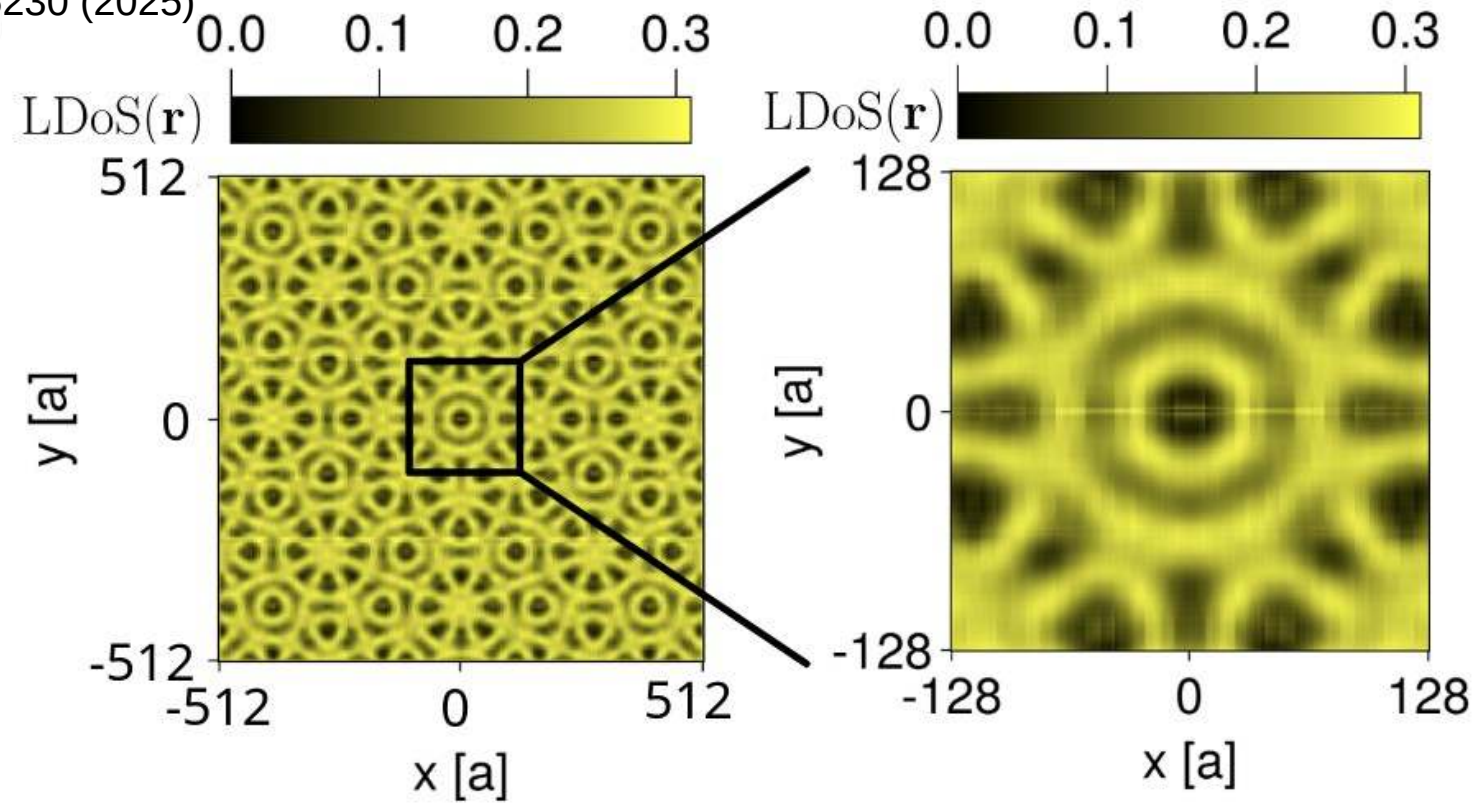
arXiv:2506.05230 (2025)



Domains with different topological invariants can be directly computed in real space

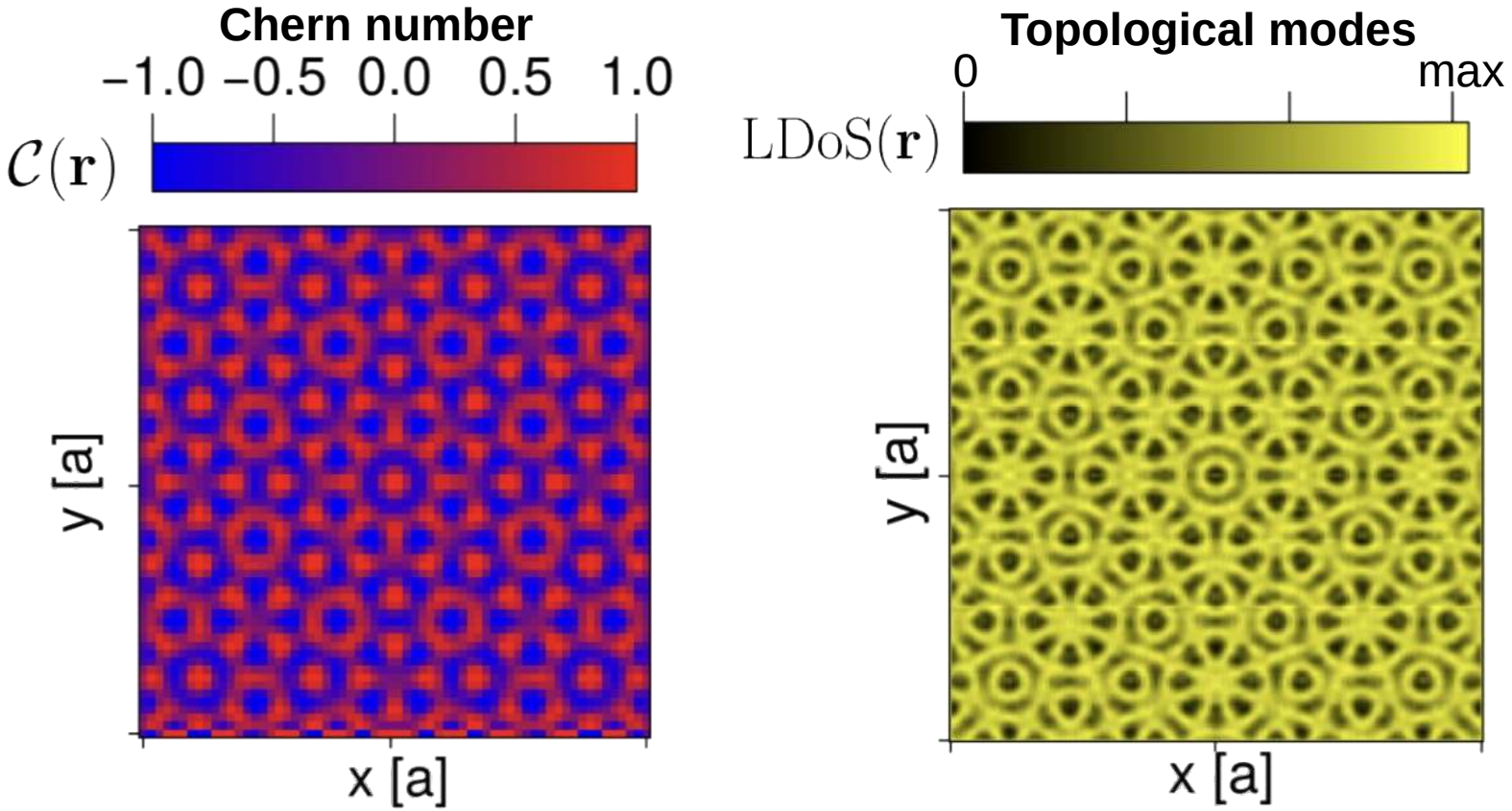
Topological modes in a 8-fold topological quasicrystal

arXiv:2506.05230 (2025)



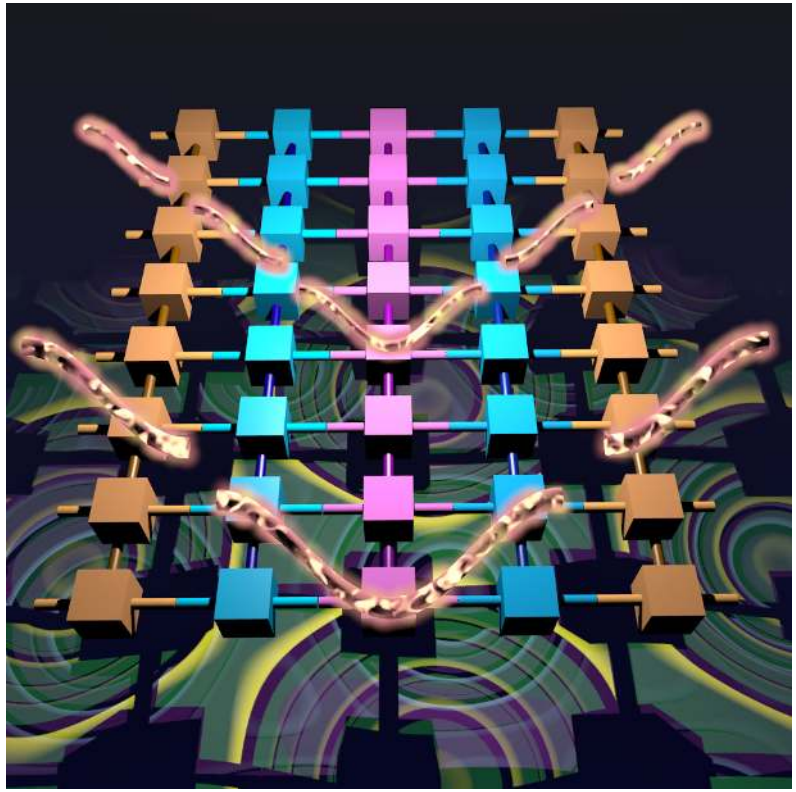
Topological modes appear between topological domains in real space

Chern mosaic and topological modes in a quasicrystal



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

Tensor networks for momentum-resolved spectral functions

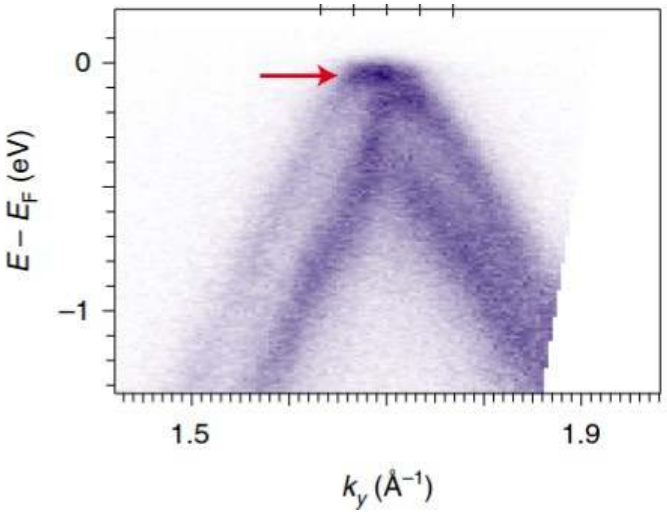


Anouar Moustaj Yitao Sun Tiago Antão

arXiv:2512.18397 (2025)

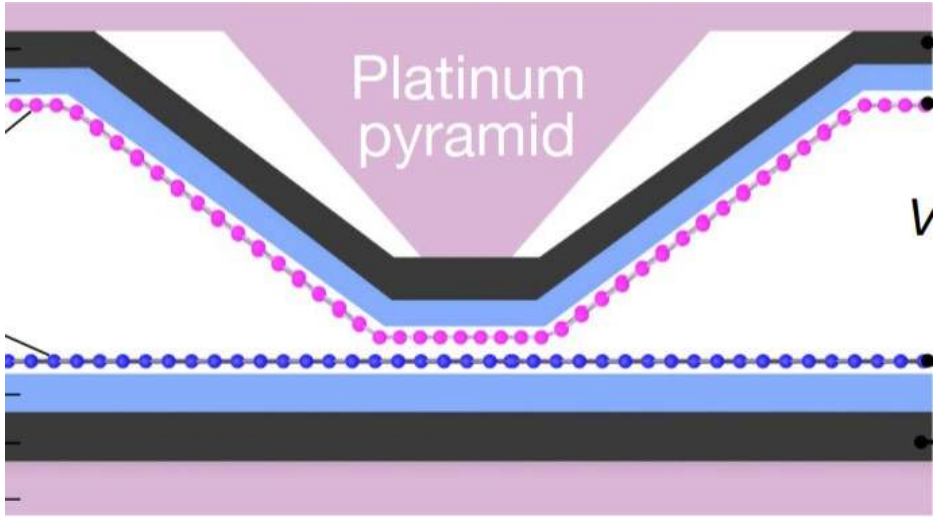
Momentum-resolved spectral functions

Angle resolved photoemission spectroscopy



Nature Physics 17, 189–193 (2021)

Quantum twisting microscope



Nature 614, 682–687 (2023)

Experiments allow accessing momentum-resolved spectral functions in different moire regions

Local momentum-resolved spectral function

Local momentum-resolved spectral function

$$A_{\mathrm{P}}(\mathbf{R},\mathbf{k},\omega) = \langle \mathbf{k}| \hat{\mathcal{F}}\hat{\mathcal{P}}_{\mathbf{R}}\delta\left(\omega - \hat{\mathcal{H}}_{\mathrm{MF}}\right)\hat{\mathcal{P}}_{\mathbf{R}}\hat{\mathcal{F}}^{-1}|\mathbf{k}\rangle$$

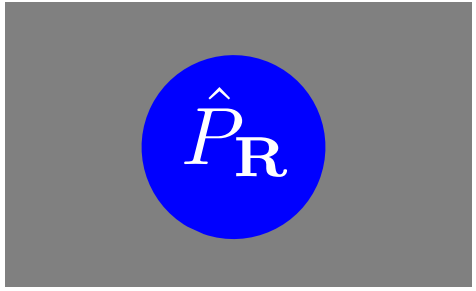
Quantum Fourier transform

Projector in a (large-enough) region

Tensor-network representation of the quantum Fourier transform

$$\hat{F}|k\rangle = \frac{1}{\sqrt{N}}\bigotimes_{r=1}^{L}\sum_{s_r=0}^{1} e^{2\pi i k s_r 2^{-r}}|s_r\rangle$$

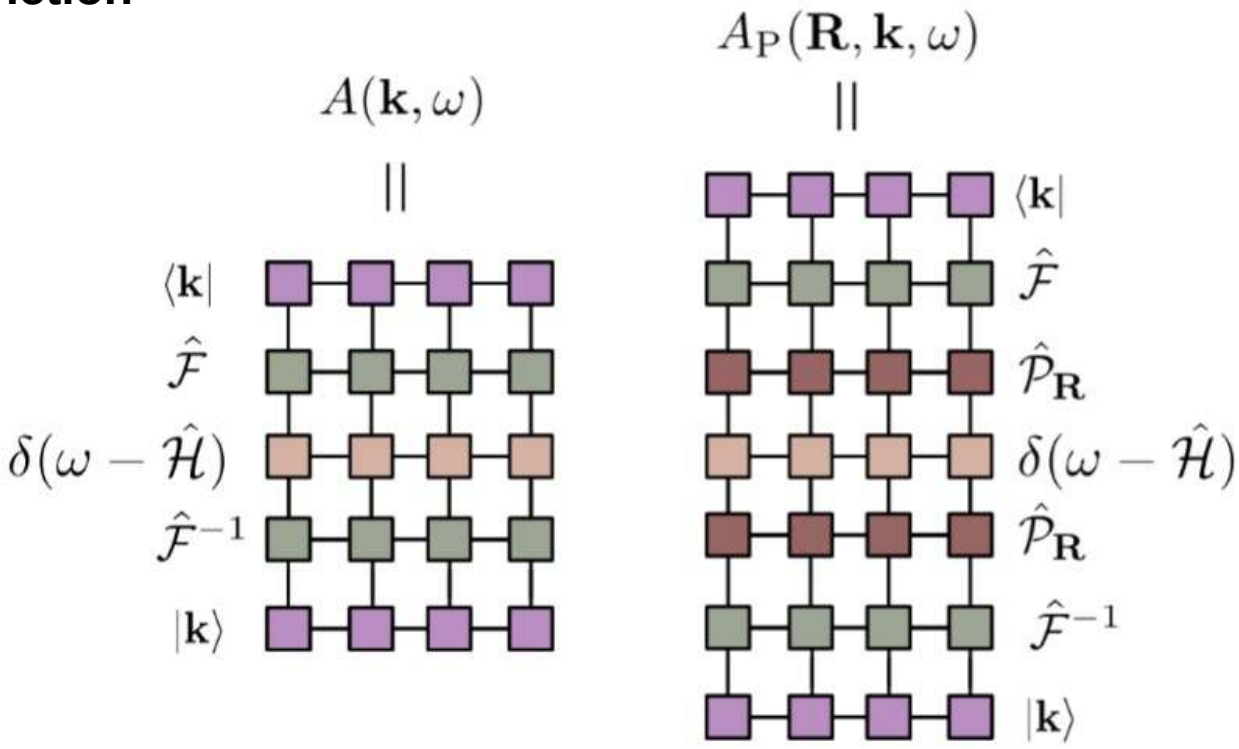
$$= \bigotimes_{r=1}^{L}\frac{1}{\sqrt{2}}\left[|0\rangle + e^{2\pi i k 2^{-r}}|1\rangle\right]$$



Tensor-network representation of the momentum-resolved spectral function

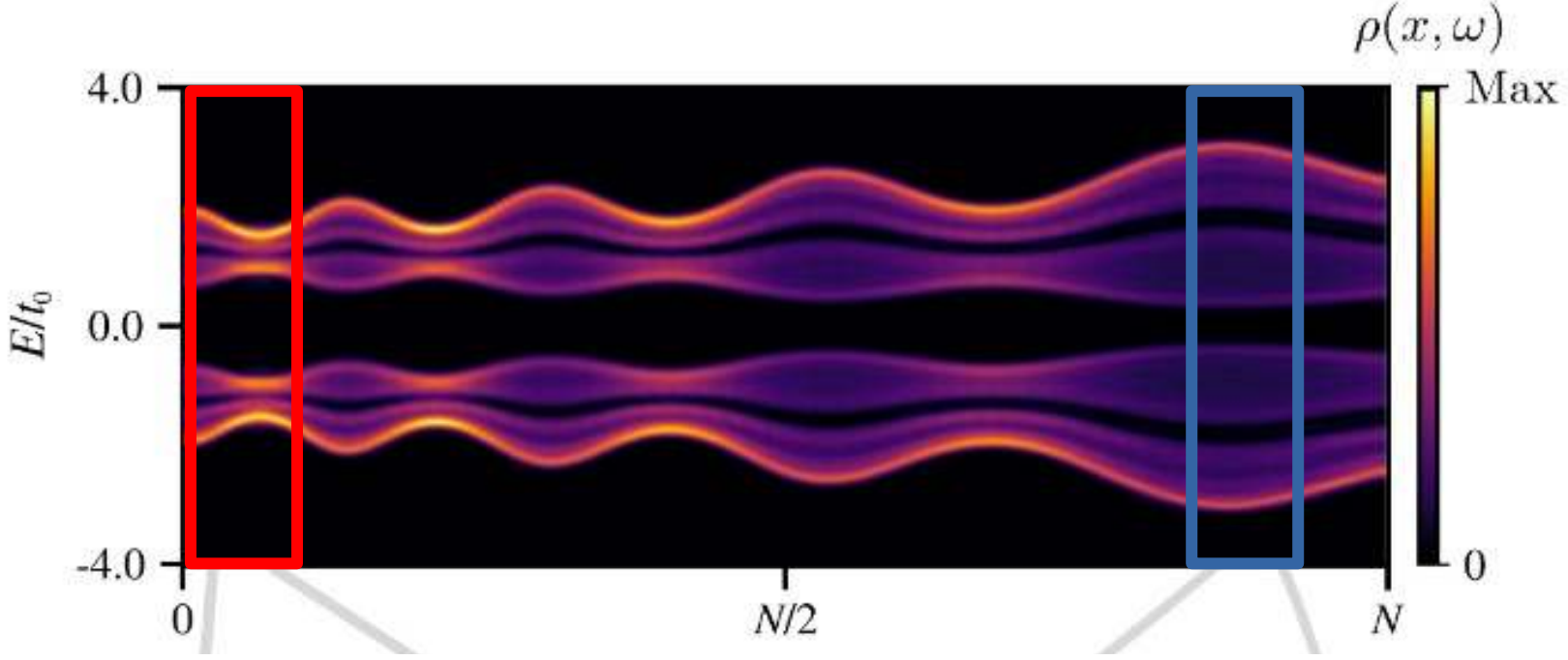
Total momentum-resolved spectral function

Local momentum-resolved spectral function



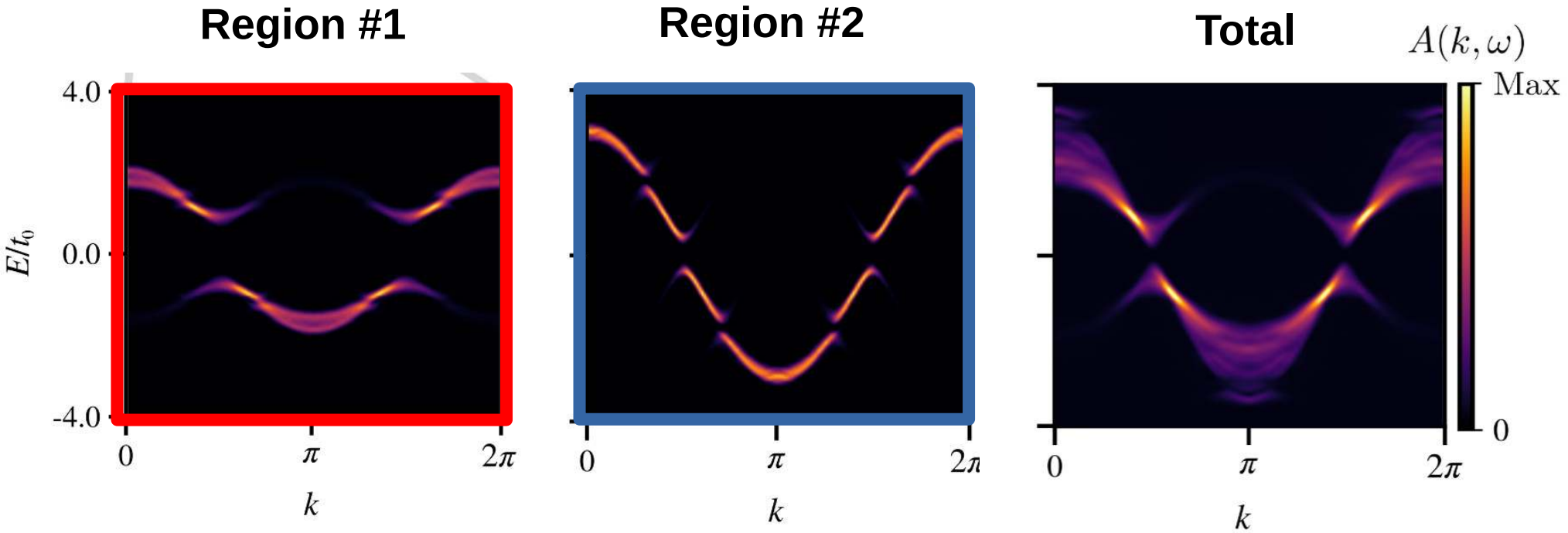
Super-moire with non-uniform strain

Super-moire system with non-uniform strain and interactions



The super-moire features a strongly spatially-dependent electronic structure, that can be imaged in the local momentum-resolved spectral function

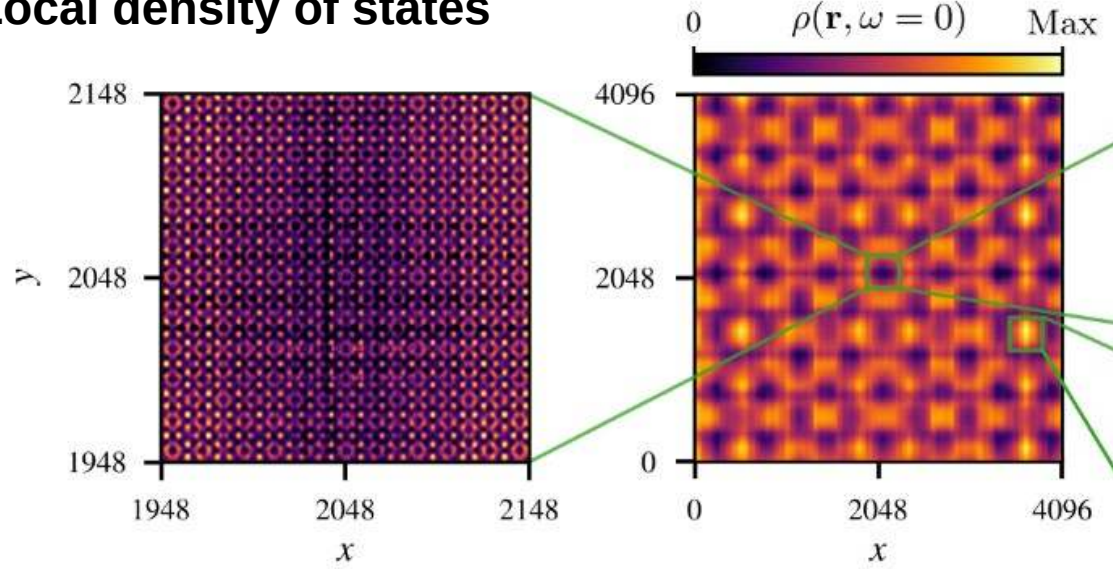
Super-moire with non-uniform strain



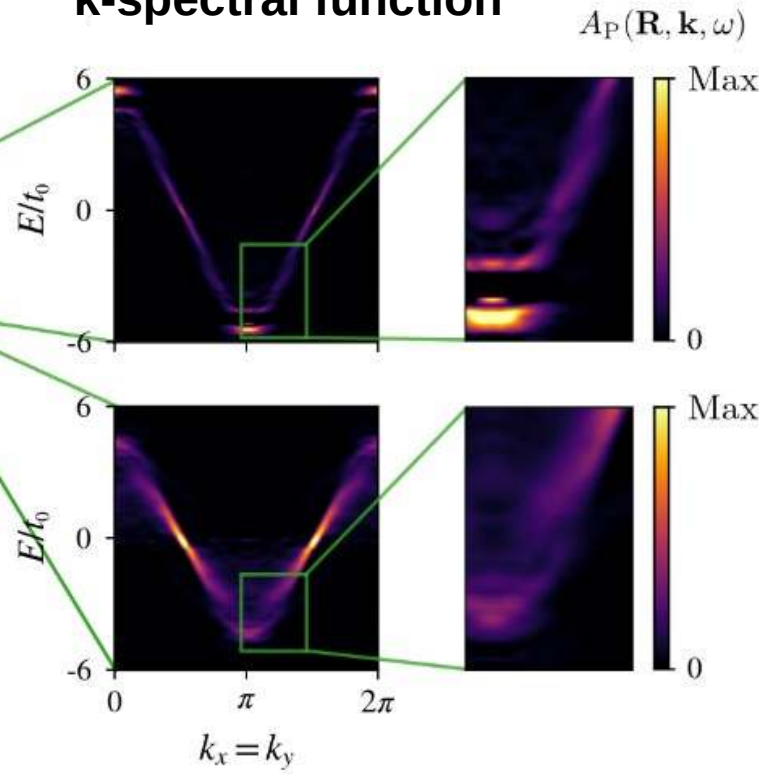
The super-moire features a strongly spatially-dependent electronic structure, that can be imaged in the local momentum-resolved spectral function

8-fold quasicrystal momentum-resolved functions

Local density of states



k-spectral function



Tensor-network momentum-resolved functions enable resolving local electronic structure I
In exceptionally large two-dimensional quasicrystals

Future of tensor networks for super-moire

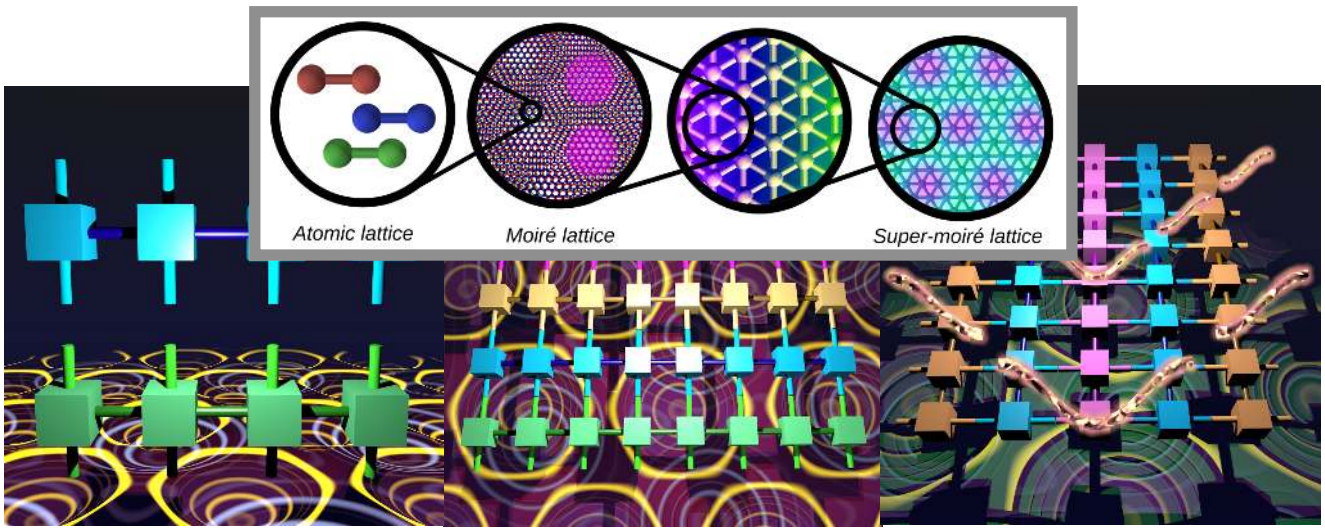
Potential future tensor network methods for super-moire

- Quantum geometry effects
- Floquet physics
- Linear and non-linear response functions
- Out of equilibrium and pump-probe
- Lateral transport, quantum twisting microscope
- General correlated symmetry broken states (valley, magnetic, CDW, SC)
- Excitons, bi-excitons, trions (arXiv:2603.02011)

Effectively, anything that was possible with tight binding models for moderate systems, but now in billion-size systems

Take home

Tensor network methods enable solving exceptionally electronic structure problems, in particular enabling reaching the scales required to model super-moire materials



Phys. Rev. Research 7, 043288 (2025)
Phys. Rev. Lett. 136, 156601 (2026)
arXiv:2512.18397 (2025)

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