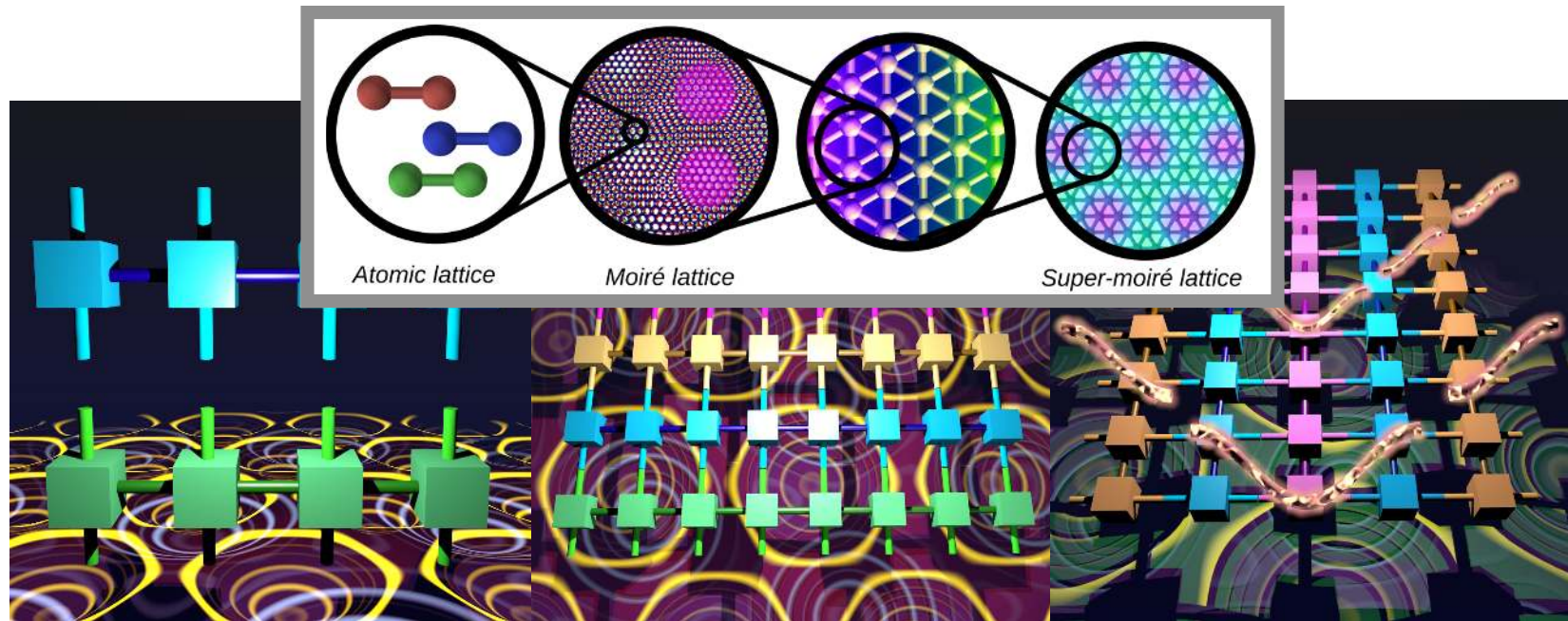


Solving topological and correlated super-moire materials beyond one billion sites with tensor networks

Jose Lado

Department of Applied Physics, Aalto University, Finland



Phys. Rev. Research 7, 043288 (2025)

arXiv:2506.05230 (2025)

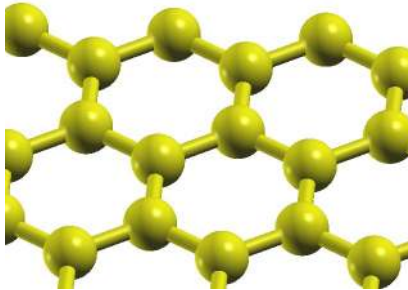
arXiv:2512.18397 (2025)

Quantum Materials in and out of Equilibrium, Bremen, February 25th 2026

The two-dimensional materials world

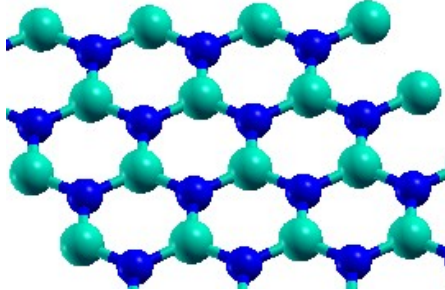
Semimetal

Graphene



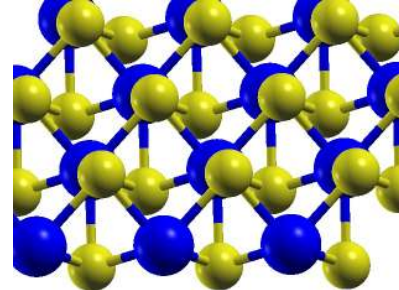
Insulator

BN



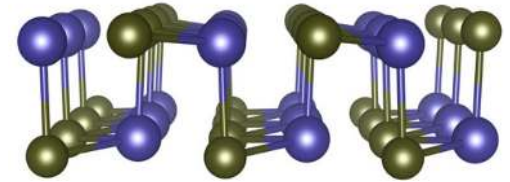
Superconductor

NbSe₂



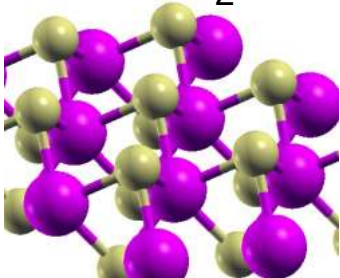
Ferroelectric

SnTe



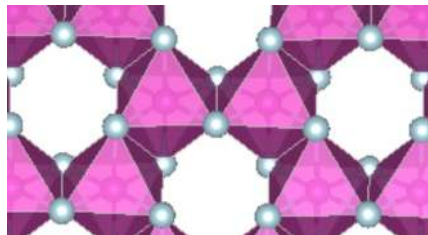
Semiconductor

WS₂



Ferromagnet

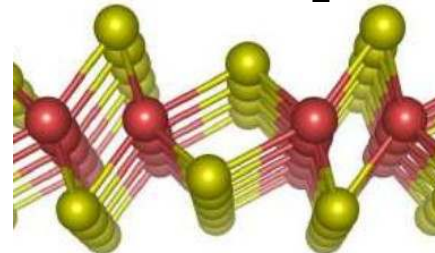
CrI₃



Quantum spin

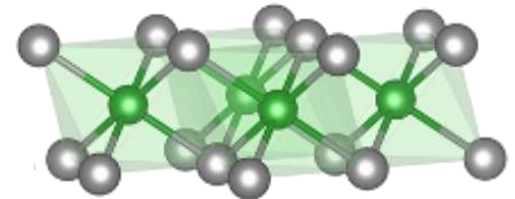
Hall insulator

WTe₂



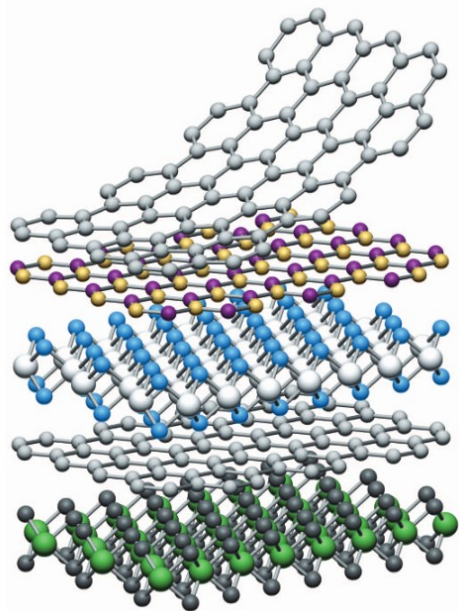
Multiferroic

NiI₂



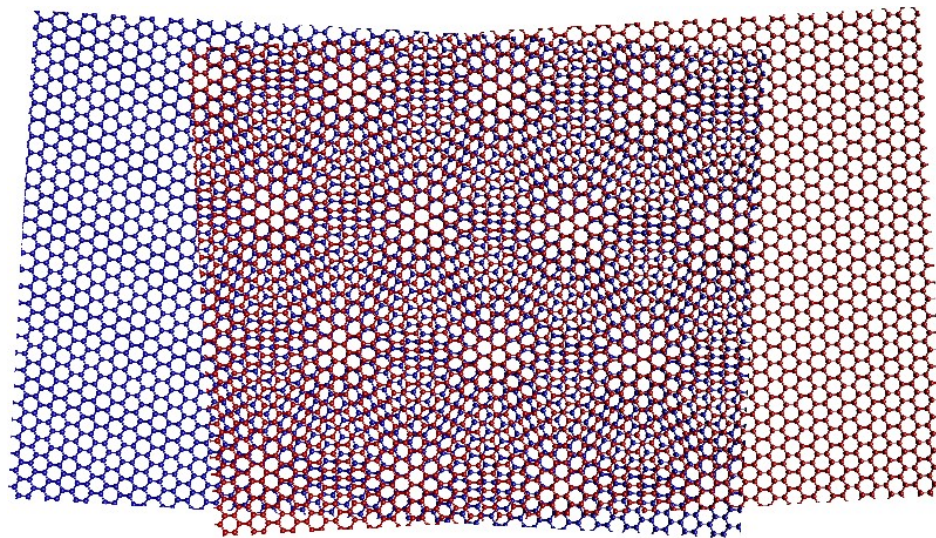
The flexibility of two-dimensional materials

They can be stacked



Nature 499, 419–425 (2013)

They can be rotated

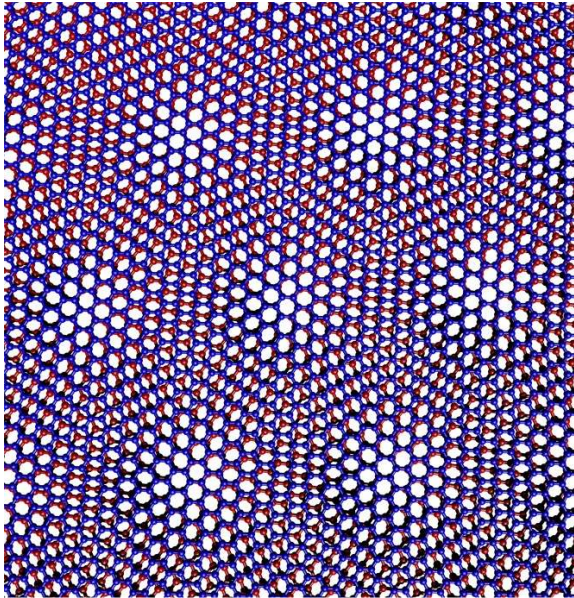


Science 361, 6403, 690-693 (2018)

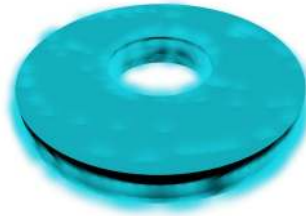
These are unique features of two-dimensional materials

The tunability of twisted van der Waals materials

Twisted bilayer graphene

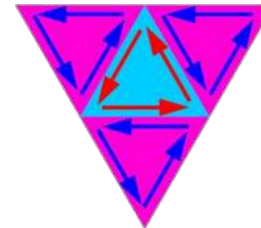


Superconductivity



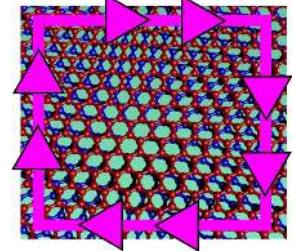
Nature 556, 43–50 (2018)

Topological networks



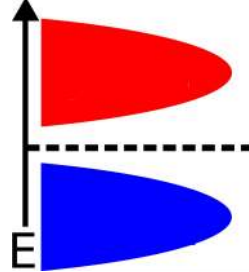
Nano Lett. 18, 11, 6725-6730 (2018)

Chern insulators



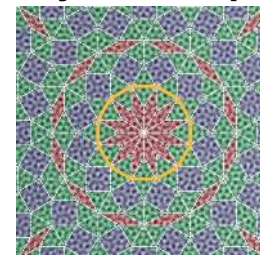
Science 365, 605-608 (2019)

Correlated insulators



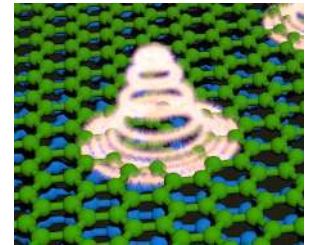
Nature 556, 80–84 (2018)

Quasicrystalline physics



Science 361, 782-786 (2018)

Proximal fractional Chern insulators

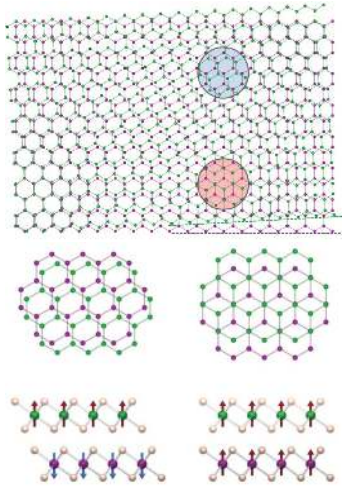


Nature 600, 439–443 (2021)

Twisted multilayers provide a powerful platform for emergent phenomena

Artificial quantum matter in moire van der Waals heterostructures

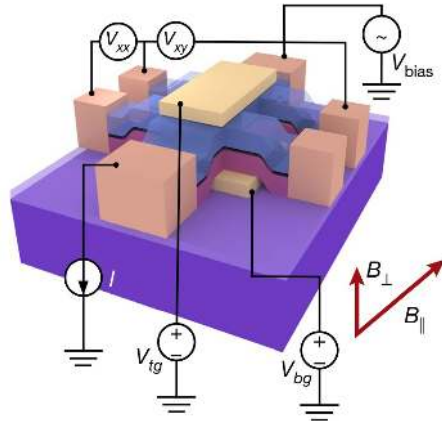
Unconventional magnets



Twisted CrBr_3

Science, 374(6571),
1140–1144 (2021)

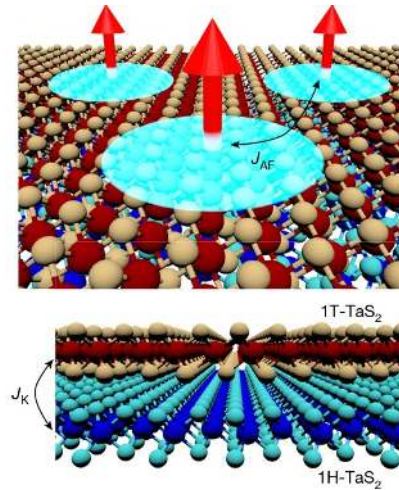
Unconventional superconductors



Twisted trilayer
graphene

Nature 595,
526–531 (2021)

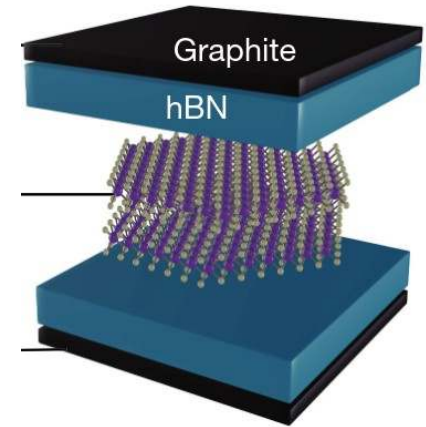
Heavy-fermion quantum materials



1H-1T TaS_2

Nature 599,
582–586 (2021)

Fractional topological matter

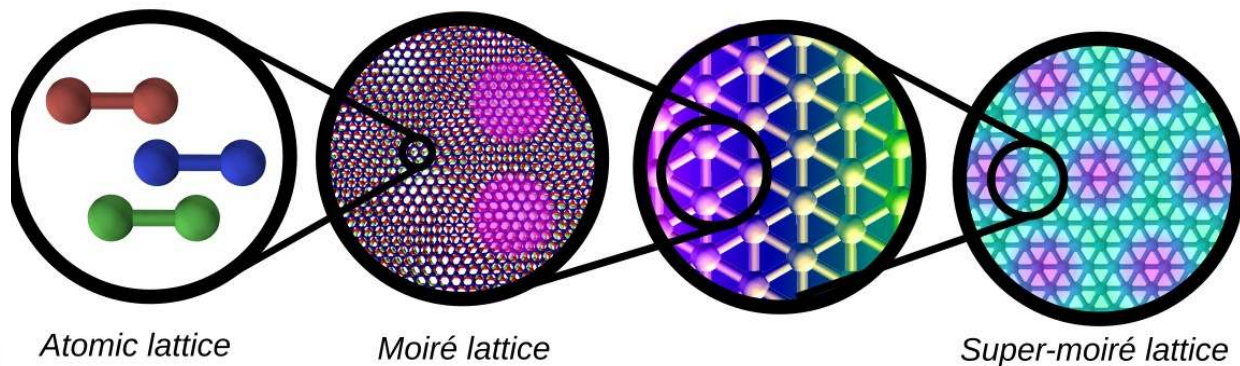
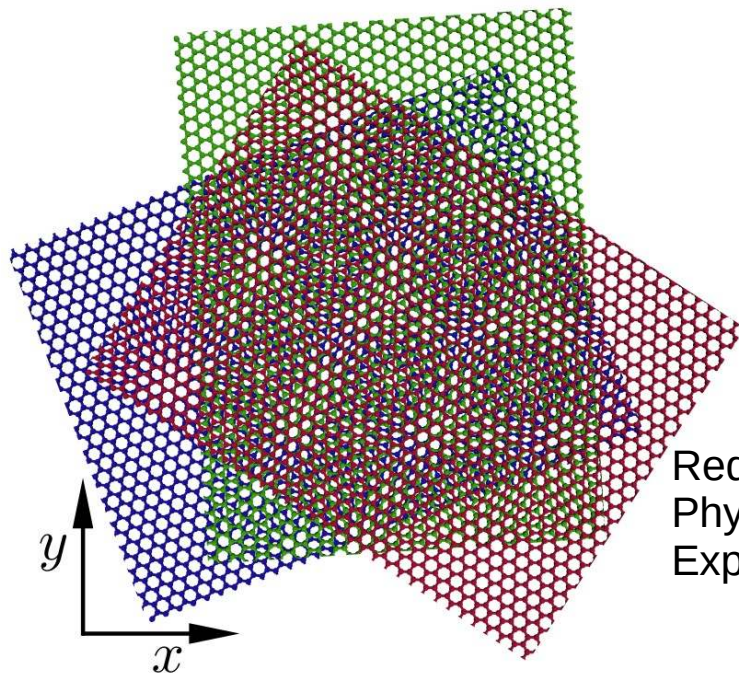


Twisted MoTe_2

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

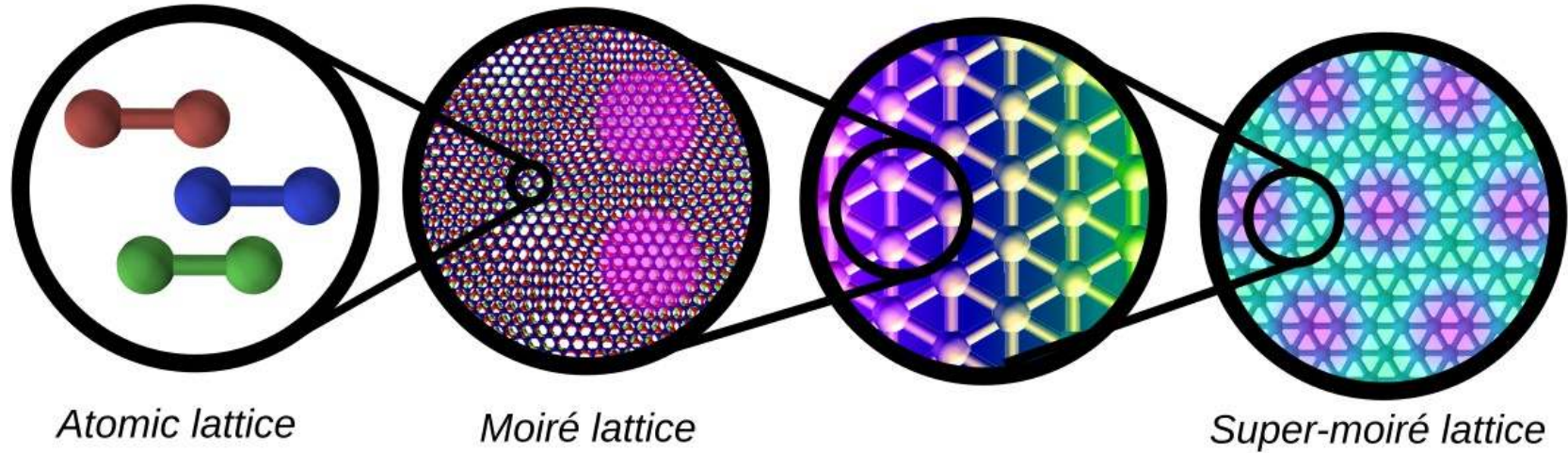
Nature 620, 762–767 (2023)

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)



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

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

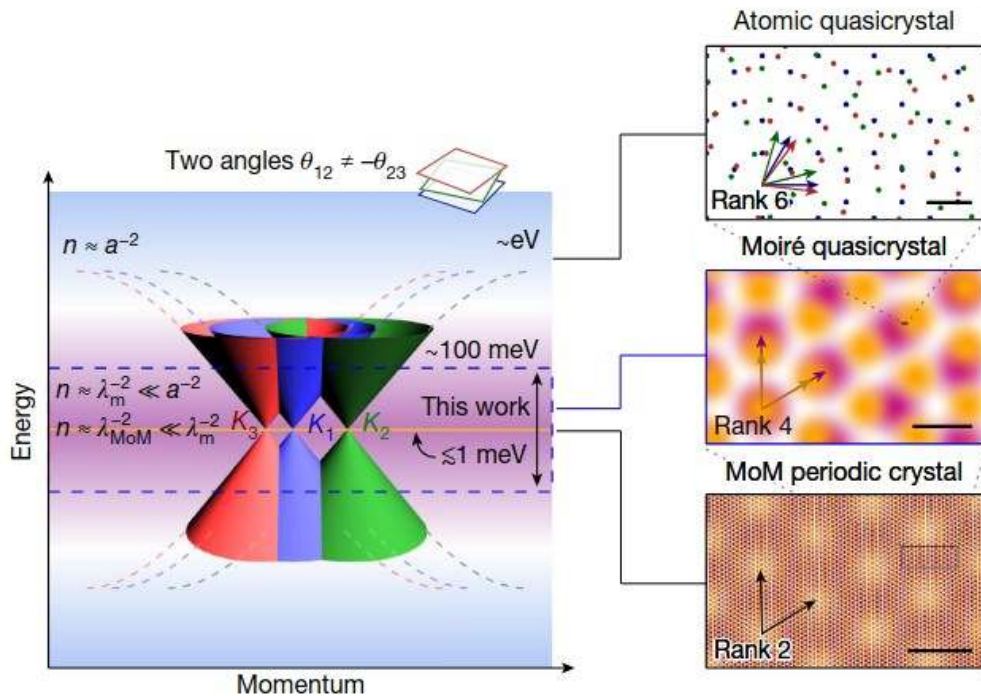
Super-moiré **$N=10^9$ sites**, calculations taking 10 days – 1000000 years

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

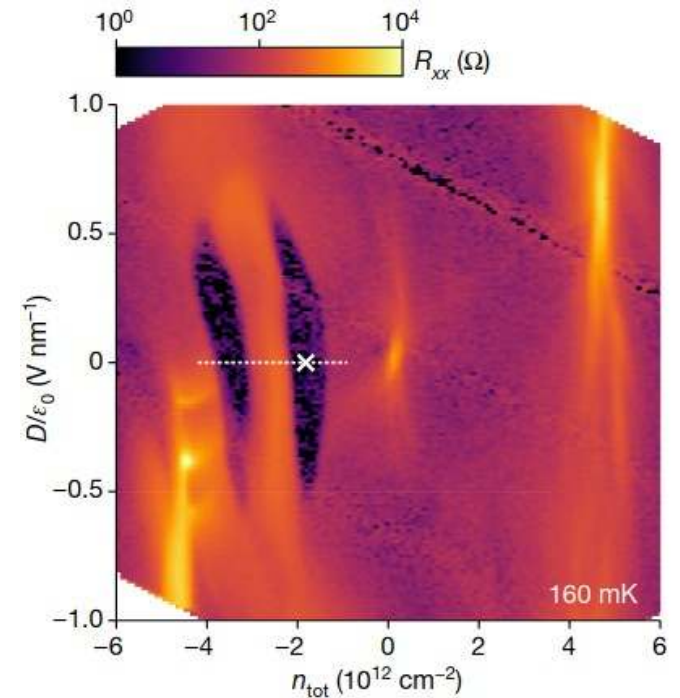
(even going beyond usual memory limitations of conventional methods)

Super-moire materials, experimentally

Moire quasicrystal in twisted trilayer graphene



Coexisting correlations and superconductivity



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, **arXiv:2506.05230** (2025)

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

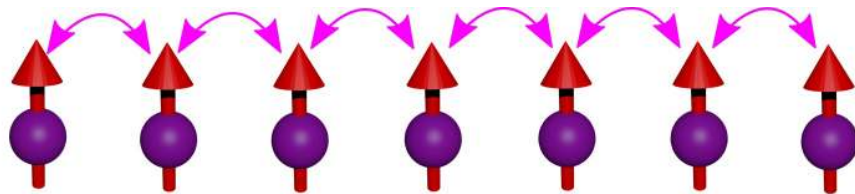
The problem of dimensionality

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

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

We need to determine in total 2^L coefficients

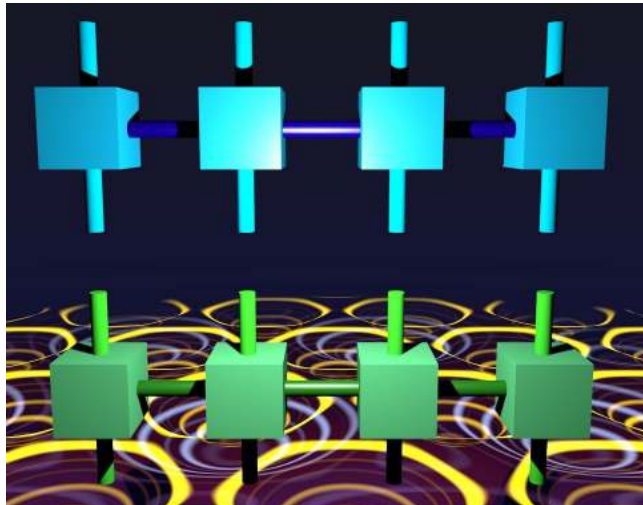
Is there an efficient way of storing so many coefficients?

Dealing with very large spaces with tensor networks

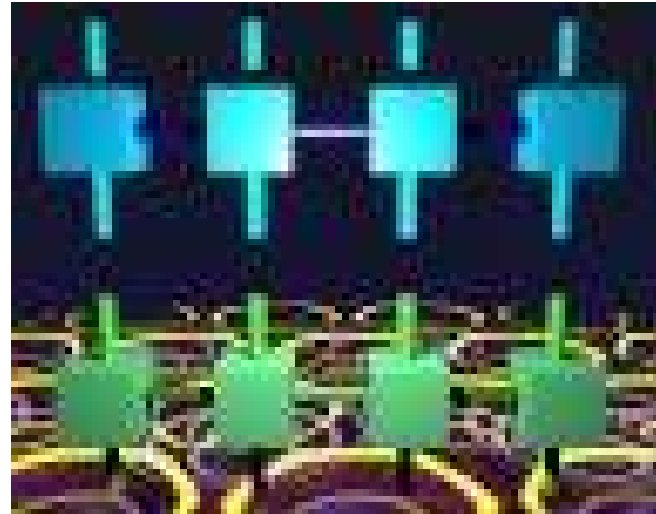
A many-body wavefunction is a very high dimensional object (2^L coefficients)

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

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



“True wavefunction”



“Tensor-network wavefunction”

Dealing with very large spaces with tensor networks

Typical many-body wavefunction

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

Tensor networks allow parametrizing many-body wavefunctions as

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

$L\chi^2$ parameters

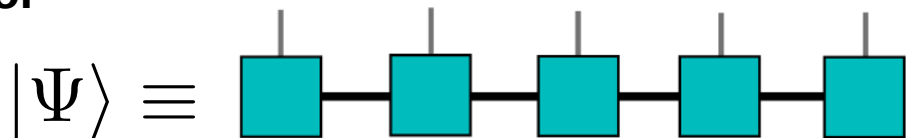


Tensor networks allow to drastically reduce the memory required to store a many-body state

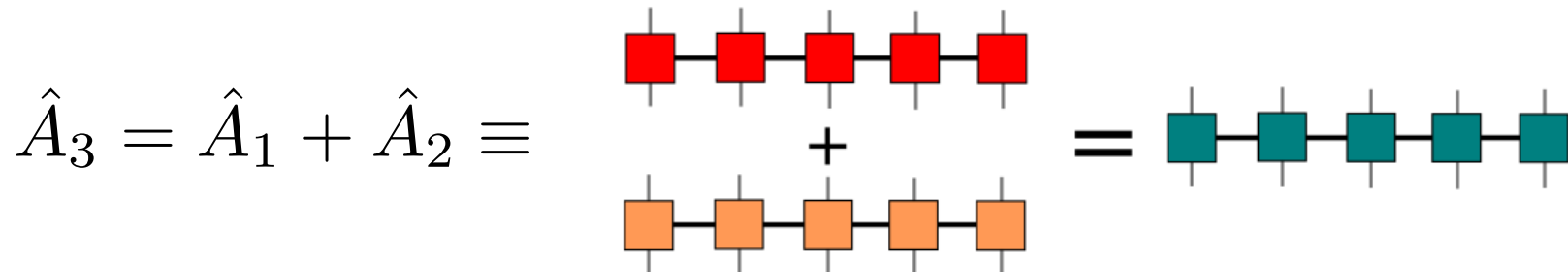
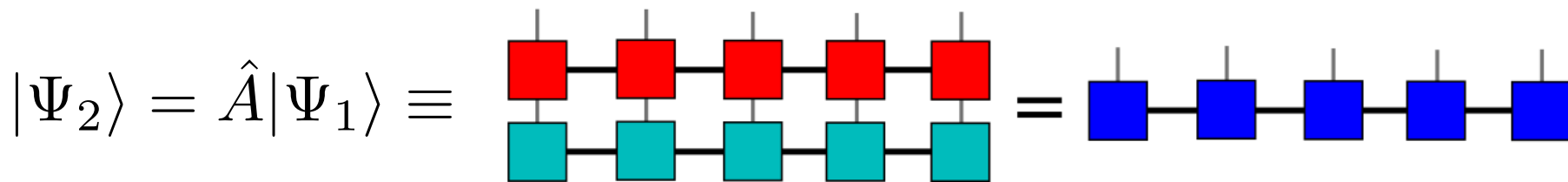
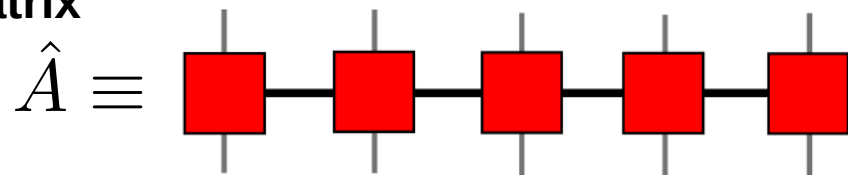
Exponentially large algebra with tensor networks

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

vector

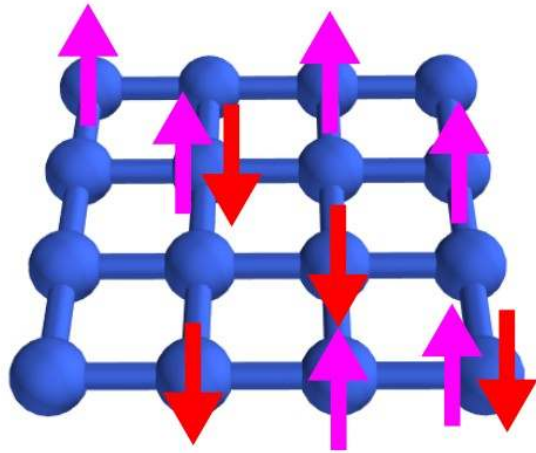


matrix



Some paradigmatic problems solved with matrix product states

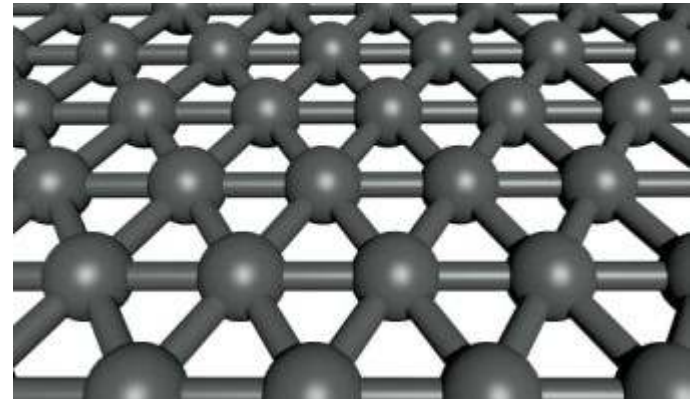
Solving the 2D Hubbard model at finite doping



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

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

Solving the 2D Heisenberg model in frustrated lattices

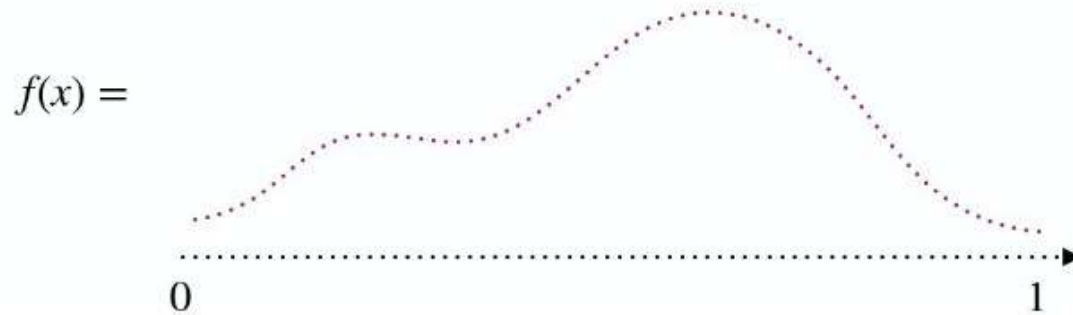


$$\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

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

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?

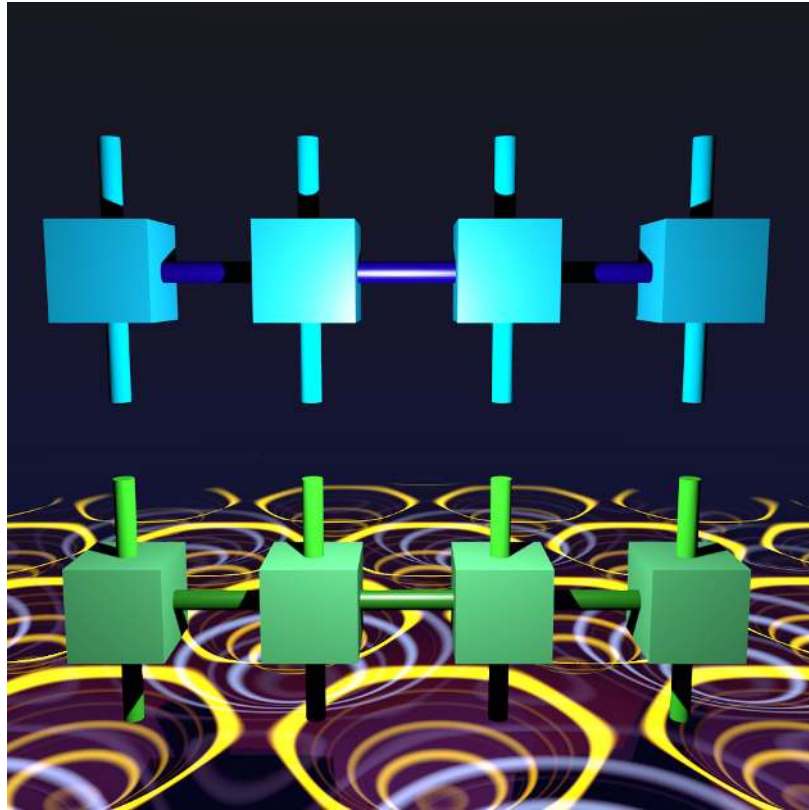
With a cross interpolation algorithm with the tensor network

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

$$\begin{pmatrix} \text{8x16 grid of colored dots} \end{pmatrix} \approx \begin{pmatrix} \text{8x4 grid of red and purple dots} \end{pmatrix} \begin{pmatrix} \text{4x4 grid of purple and white dots} \end{pmatrix}^{-1} \begin{pmatrix} \text{8x12 grid of blue and purple dots} \end{pmatrix}$$

Quantum inspired active learning to learn exponentially large spaces

Tensor-networks for interacting super-moire materials



Phys. Rev. Research 7, 043288 (2025)

Yitao Sun



Marcel
Niedermeier



Tiago Antão



Adolfo
Fumega



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

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

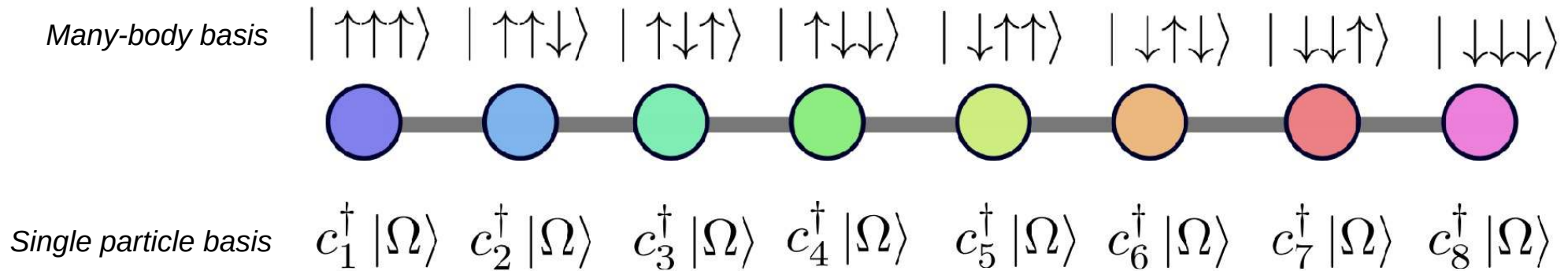
Solving the system requires dealing with matrices proportional to the system size

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



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: **a quantum-inspired active learning algorithm***

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

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

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

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

$$\mathcal{H}_{\alpha\beta}^{MF} \equiv \text{[Diagram: A chain of orange squares connected by horizontal lines, representing a tensor network for the mean-field Hamiltonian.]}$$

Chebyshev expansion of the correlators

$$\langle c_{\alpha}^{\dagger} c_{\beta} \rangle = \langle \alpha | \Xi(\mathcal{H}^{MF}) | \beta \rangle \equiv \text{[Diagram: A chain of cyan squares connected by horizontal lines, representing the Chebyshev expansion of the correlator.]}$$

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

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

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

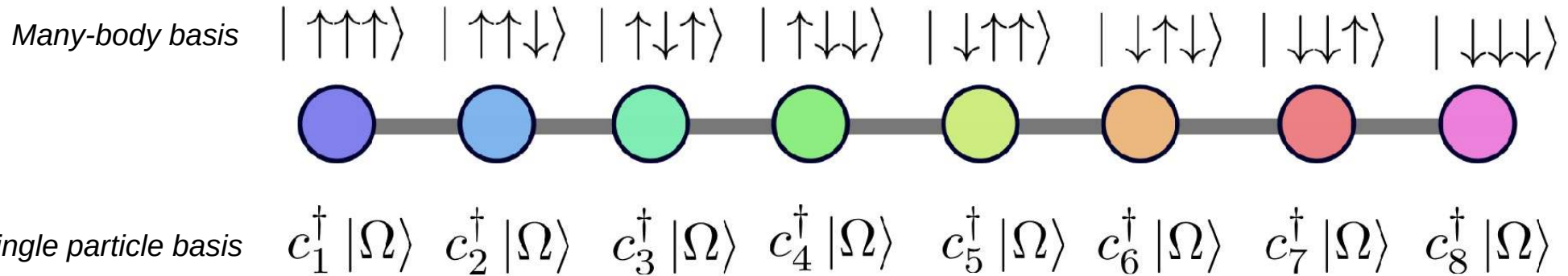
$$P_n(\omega) = \frac{2T_n(\omega)}{\pi\sqrt{1-\omega^2}}$$

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

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

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

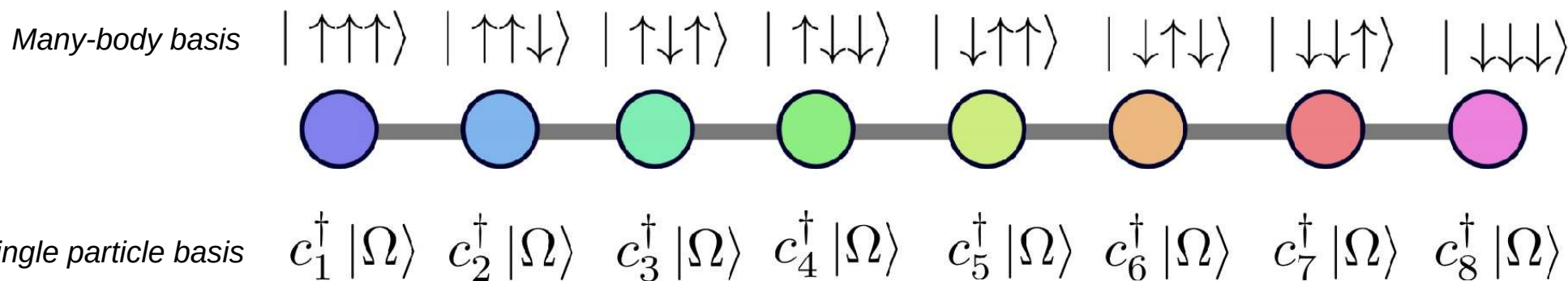
$$H_{0,NN} = \sum_{\alpha,s}^{N-1} t(c_{x_{\alpha+1},s}^{\dagger} c_{x_{\alpha},s} + h.c.)$$

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 $\mathcal{T}$

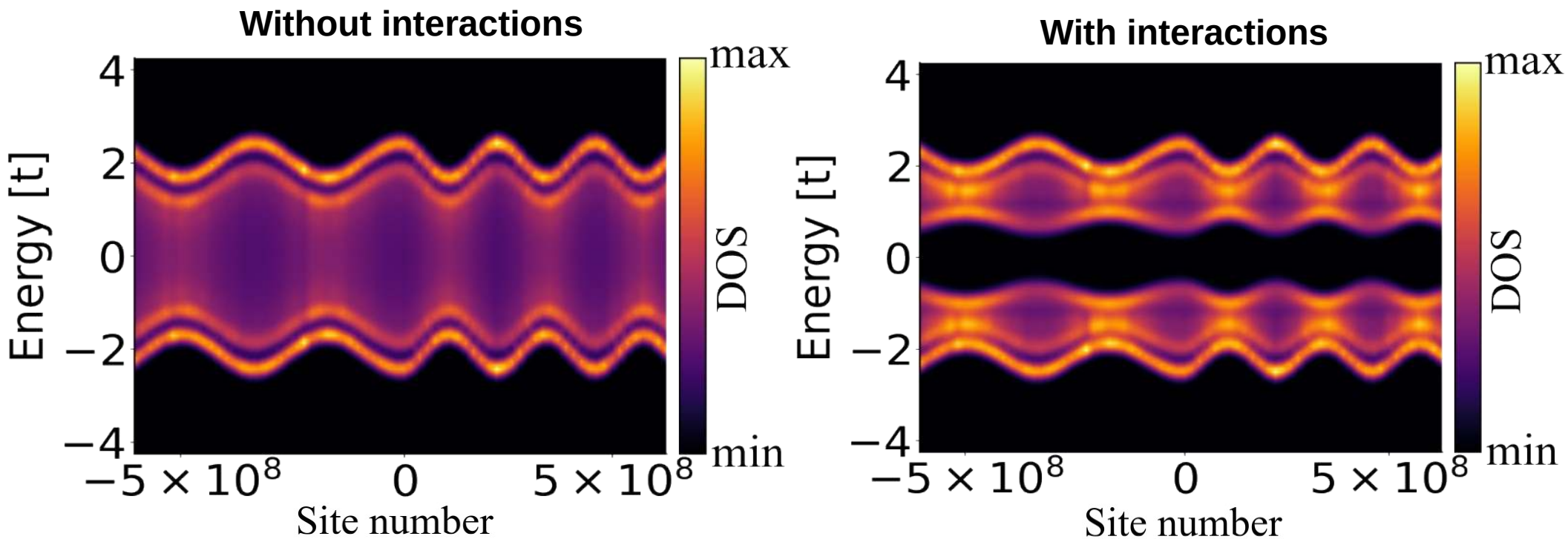
$$|\tau\rangle = \sum M_{s_1}^{(1)} M_{s_2}^{(2)} M_{s_3}^{(3)} \dots M_{s_L}^{(L)} |s_1, s_2, \dots, s_L\rangle$$

Quantics tensor cross interpolation

Modulated super-moire by construction

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

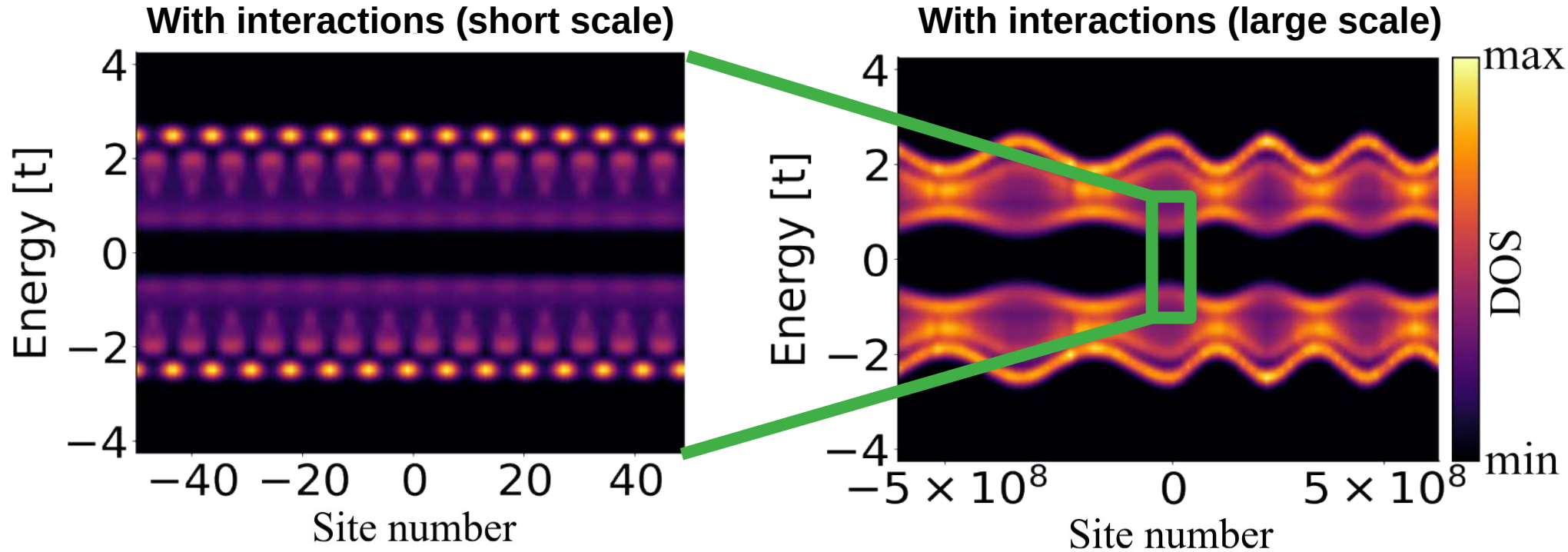
Solving billion-size super-moire materials



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

Phys. Rev. Research 7, 043288 (2025)

Solving billion-size super-moire materials

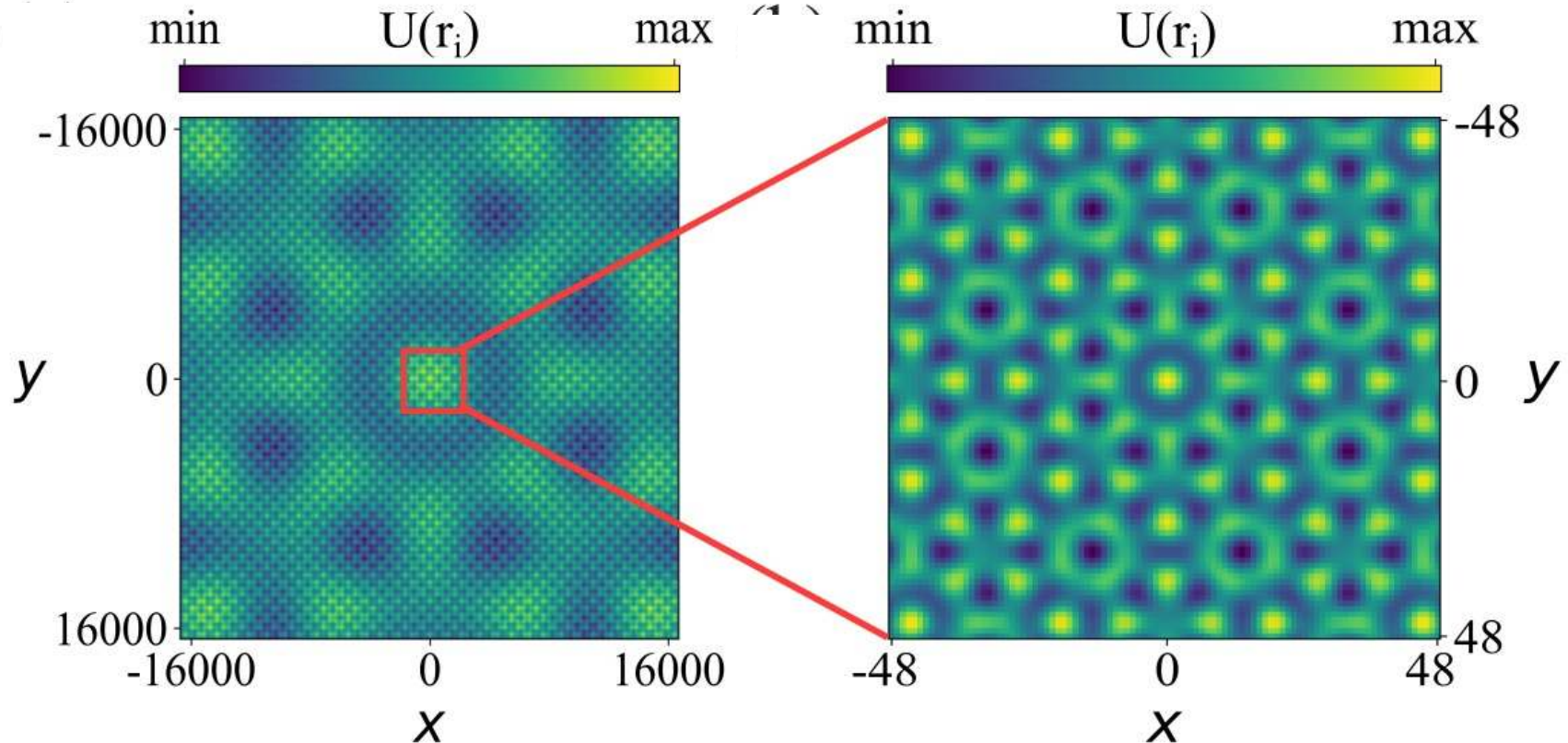


Tensor networks allow to solve selfconsistently a super-moire with one billion sites

Phys. Rev. Research 7, 043288 (2025)

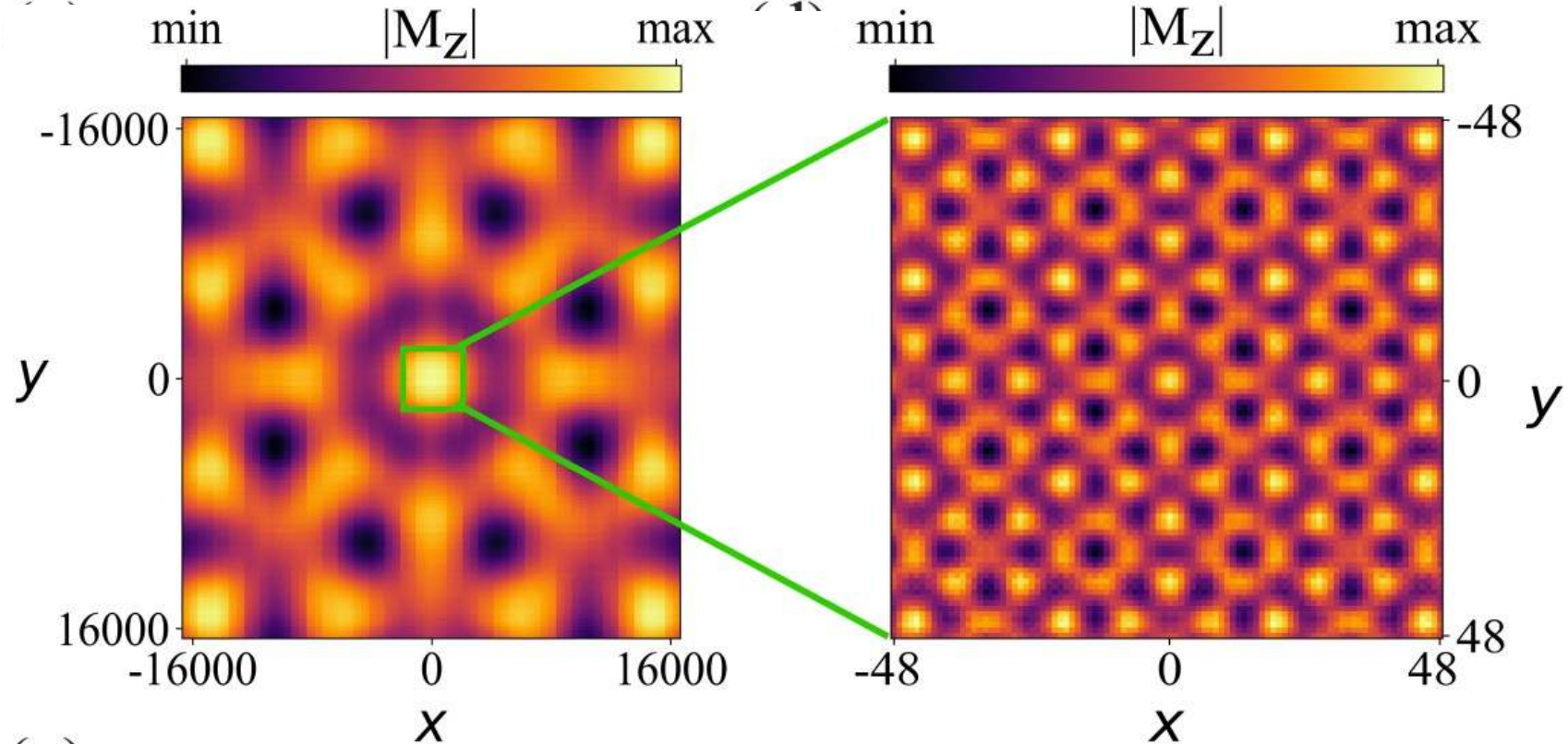
Two-dimensional billion size interacting super-moire

Modulation to the Hamiltonian



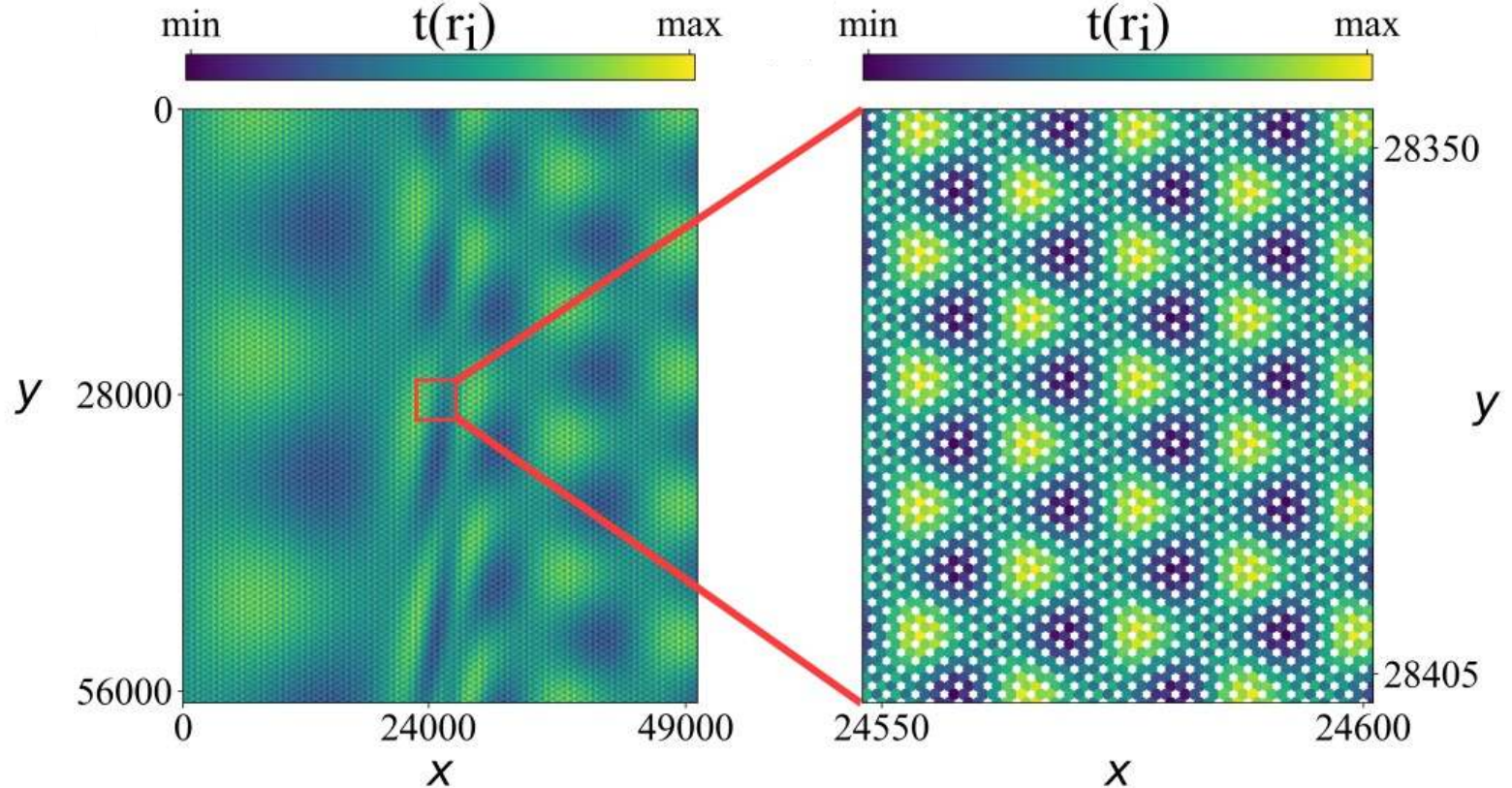
Two-dimensional billion size interacting super-moire

Selfconsistent symmetry broken order (magnetization)



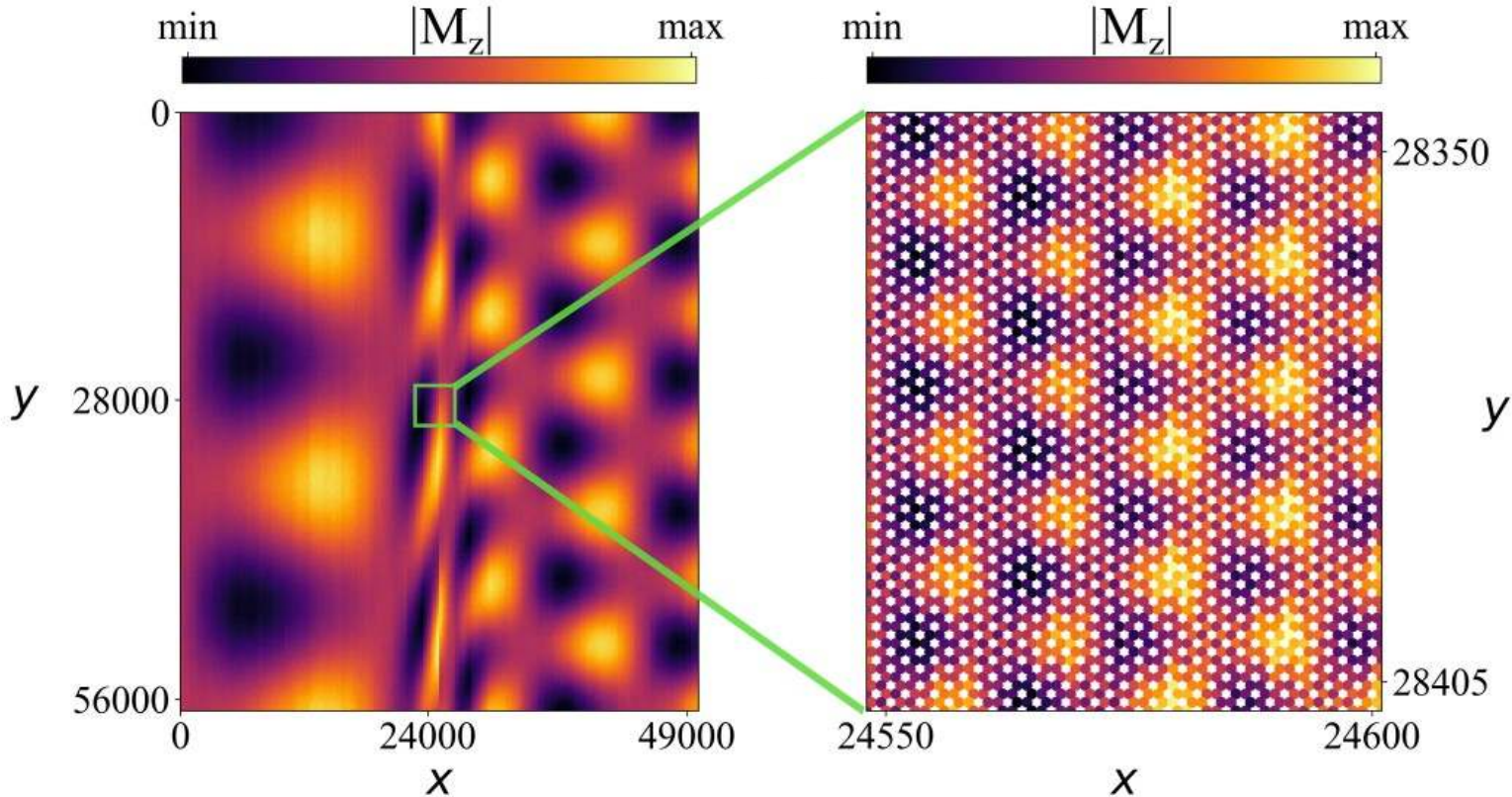
Two-dimensional billion size interacting super-moire

Modulation fo the Hamiltonian

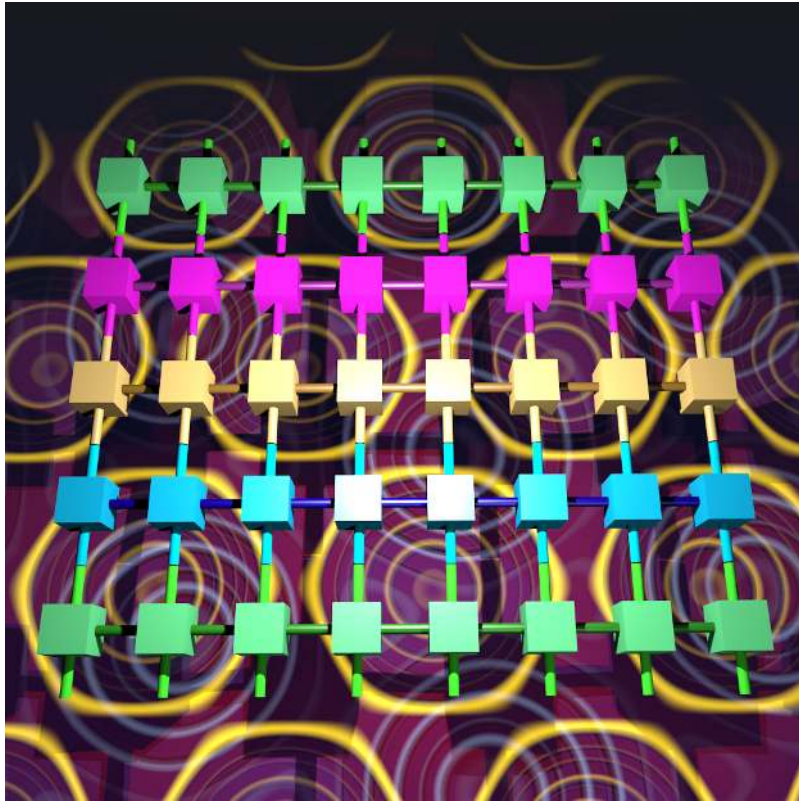


Two-dimensional billion size interacting super-moire

Selfconsistent symmetry broken order (magnetization)



Tensor networks for topological super-moire materials



Yitao Sun



Tiago Antão



Adolfo
Fumega



arXiv:2506.05230 (2025)

Topological invariant in a Hamiltonian

We can classify Hamiltonians according to topological invariants

Hamiltonian

$$H(\mathbf{k})$$

Wavefunction

$$|\Psi(\mathbf{k})\rangle$$

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

Topological invariant
(Chern number)

$$\Omega = \nabla \times \mathbf{A}|_z$$

Metric
(Berry curvature)

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

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

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

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

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

Kernel polynomial for topological invariants in real-space

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

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

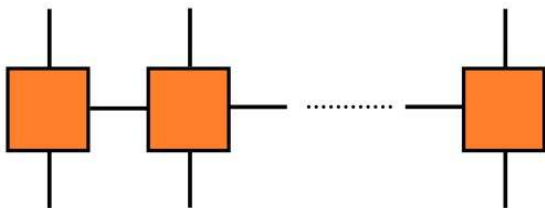
With a kernel polynomial tensor network algorithm

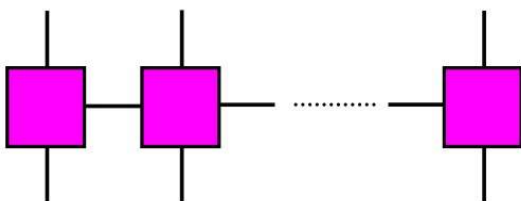
$$\hat{\mathcal{P}} = \sum_n T_n(\hat{\mathcal{H}}) \int_{-\infty}^{\varepsilon_F} d\omega \frac{T_n(\omega)}{\sqrt{1 - \omega^2}},$$

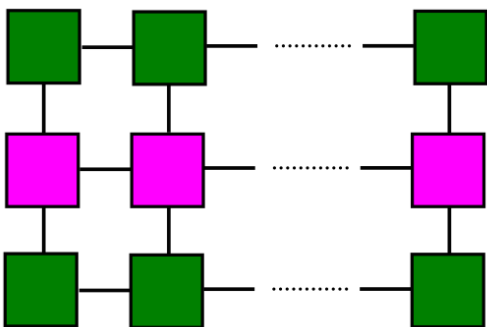
$$T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x)$$

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

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)

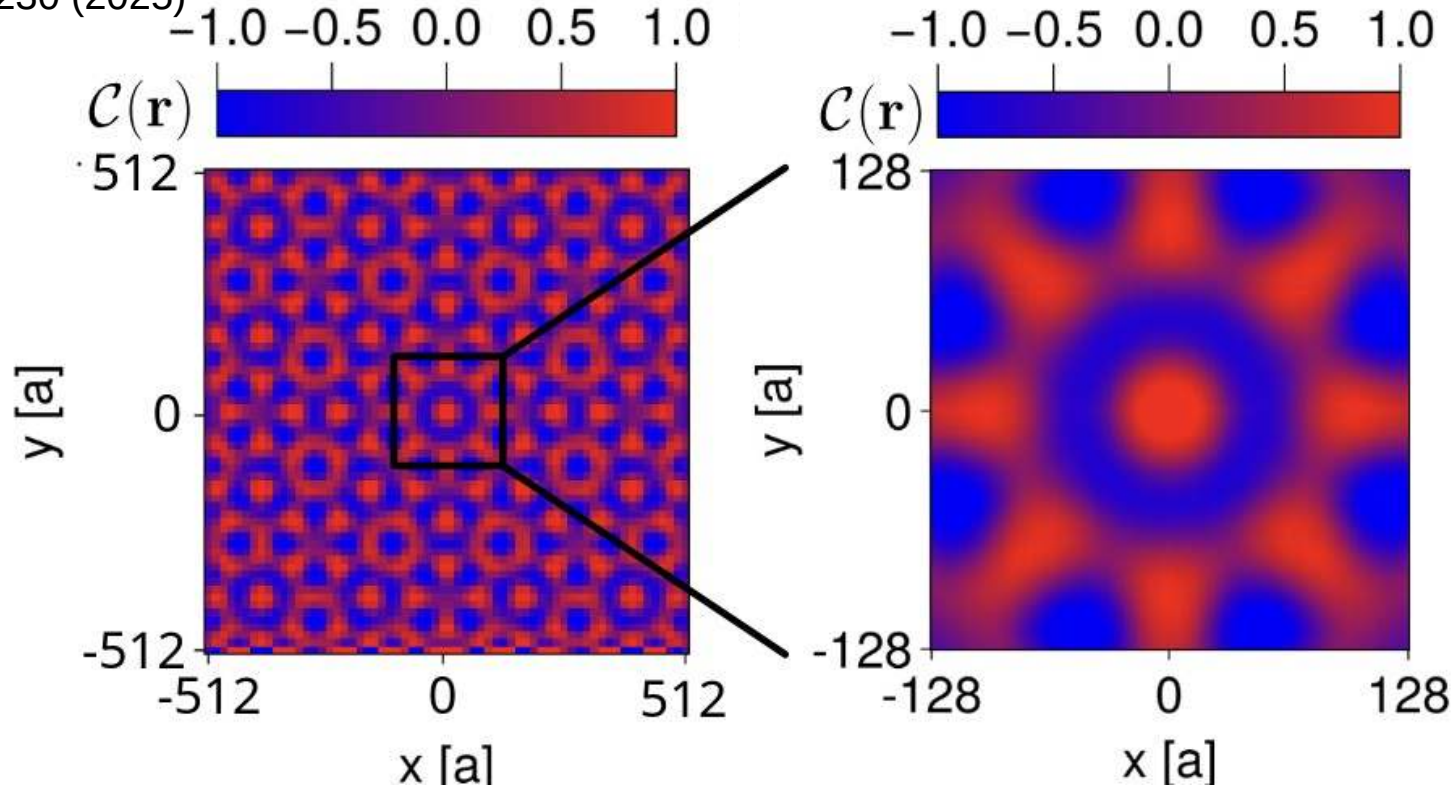
$$C_{\alpha} = 2\pi i \langle \alpha | \hat{Q} \hat{X} \hat{P} \hat{Y} \hat{Q} - \hat{P} \hat{X} \hat{Q} \hat{Y} \hat{P} | \alpha \rangle$$

Tensor-network Chern marker

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

Chern mosaic in a 8-fold topological quasicrystal

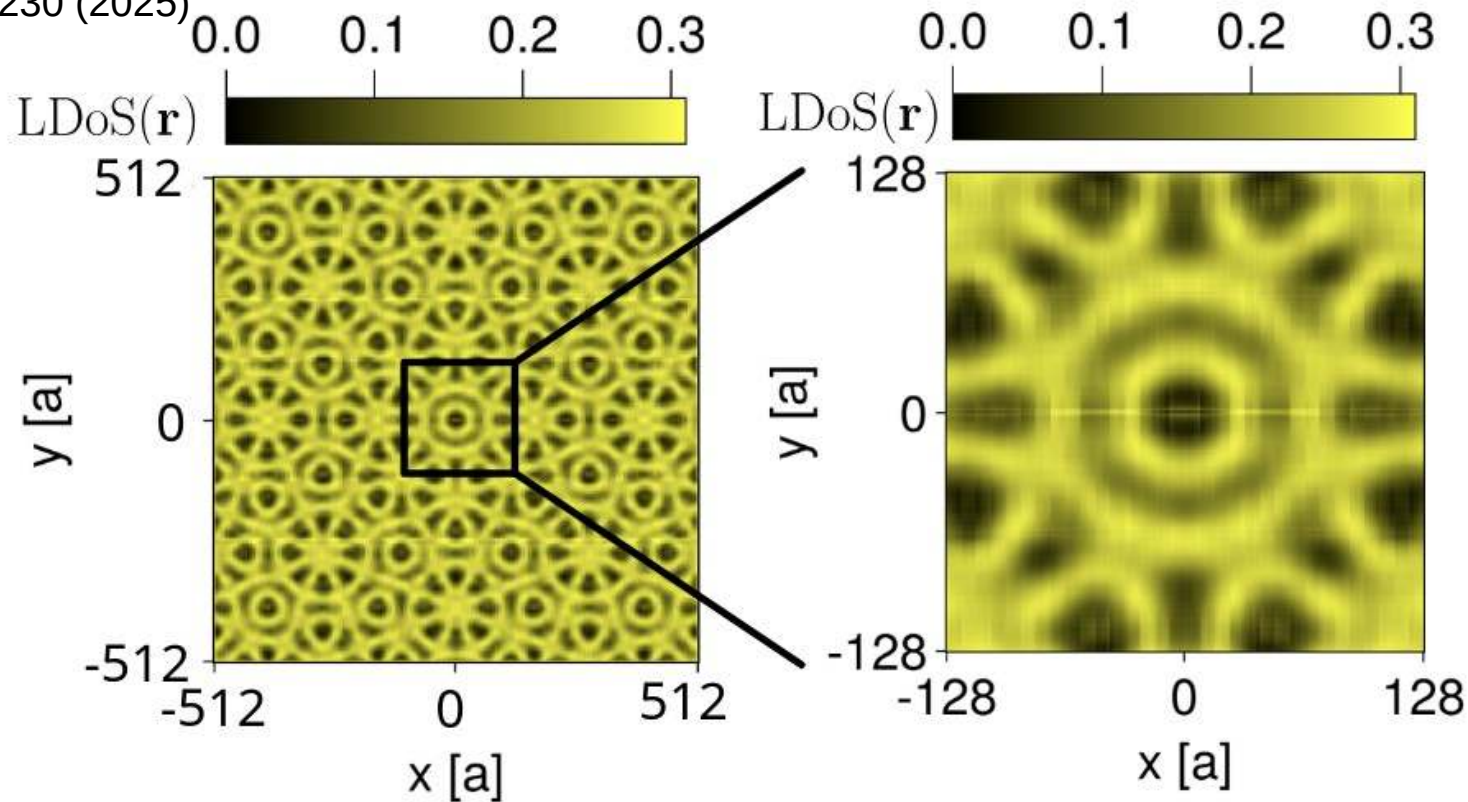
arXiv:2506.05230 (2025)



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

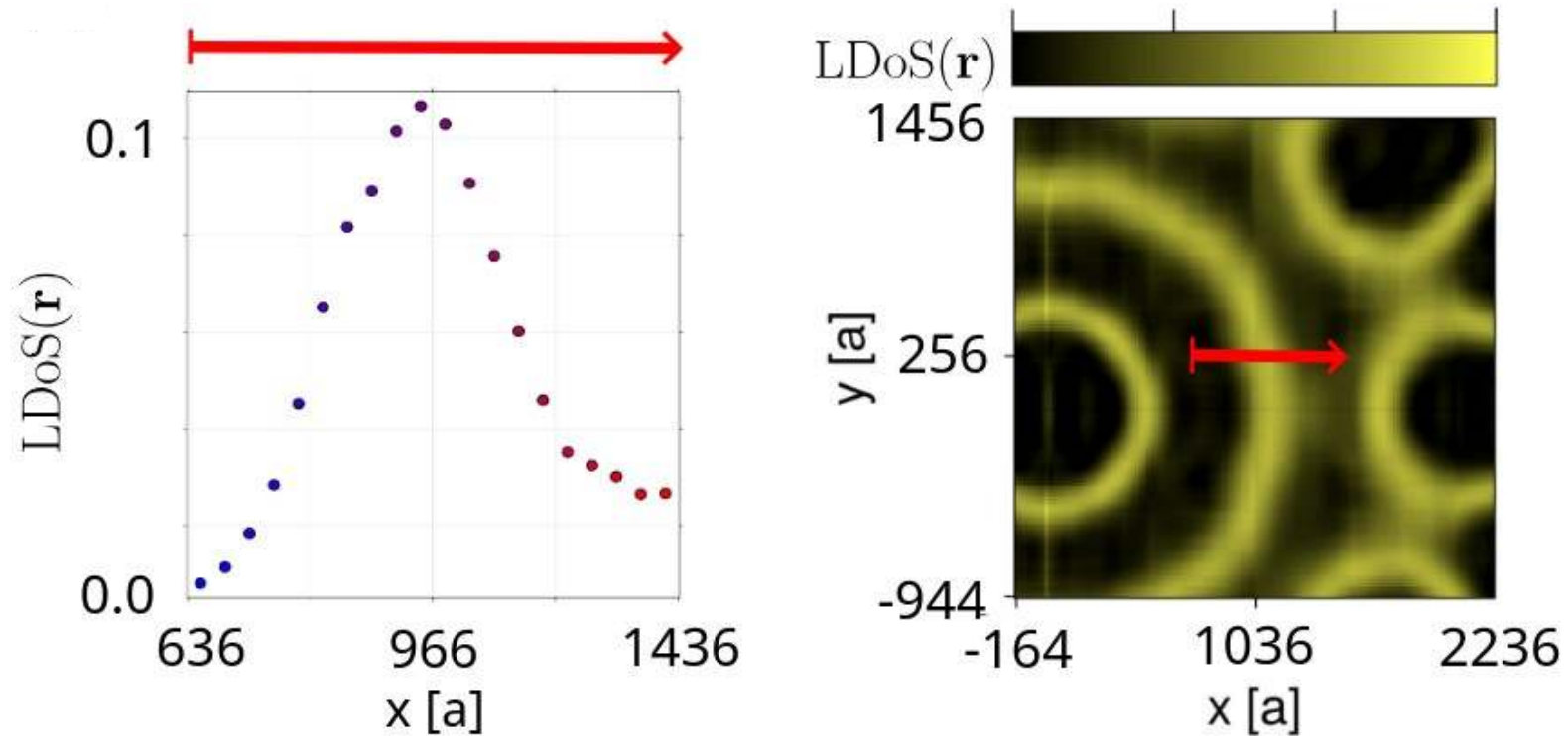
Topological modes in a 8-fold topological quasicrystal

arXiv:2506.05230 (2025)



Topological modes appear between topological domains in real space

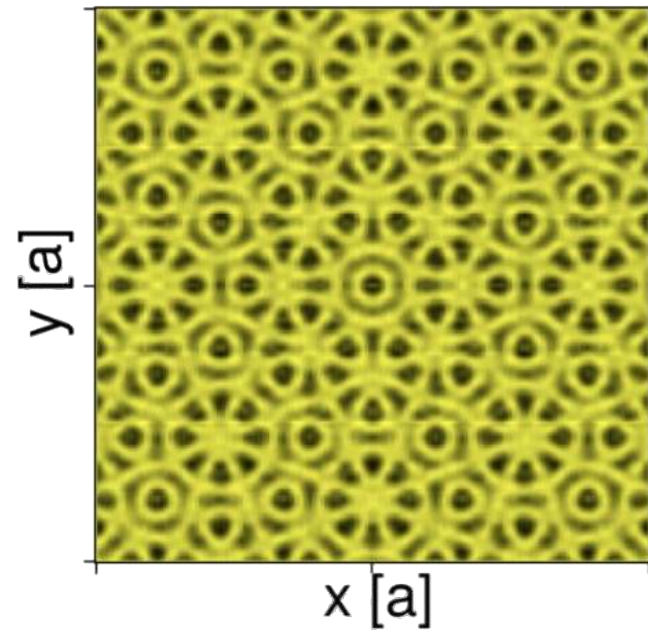
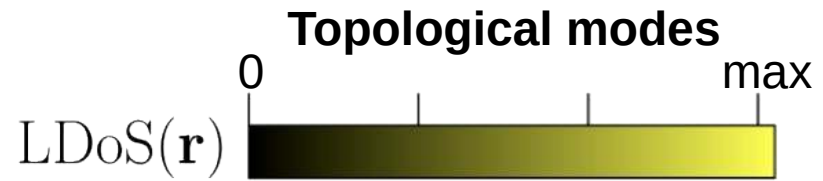
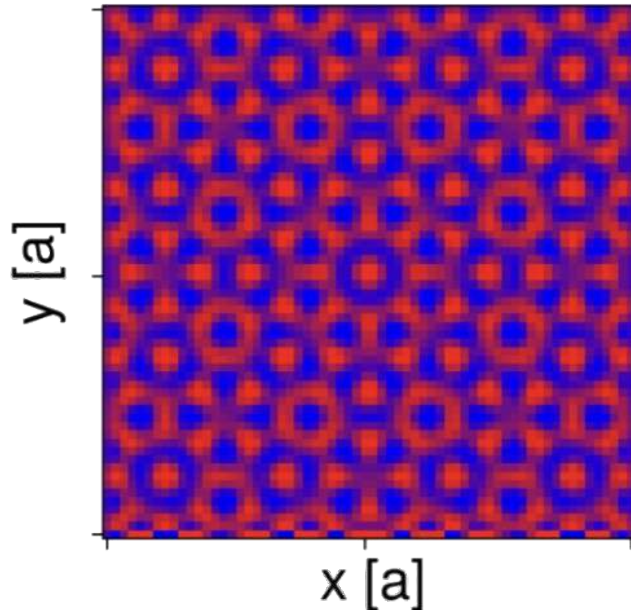
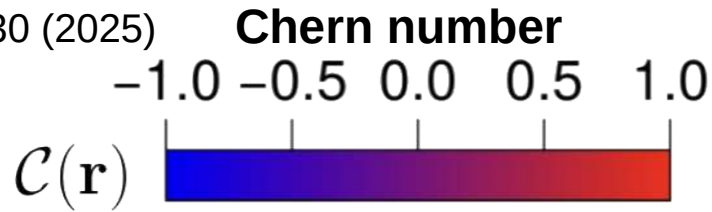
Zero modes across topological quasicrystalline domain



The real space distribution of topological states can be mapped in real space

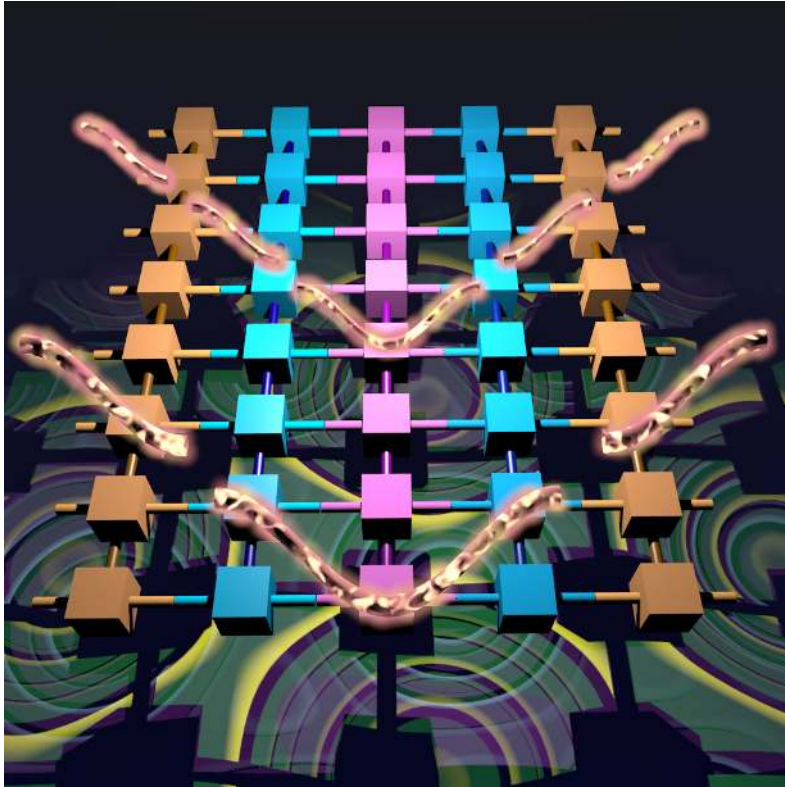
Chern mosaic and topological modes in a quasicrystal

arXiv:2506.05230 (2025)



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

Tensor networks for momentum-resolved spectral functions



Anouar Moustaj



Yitao Sun



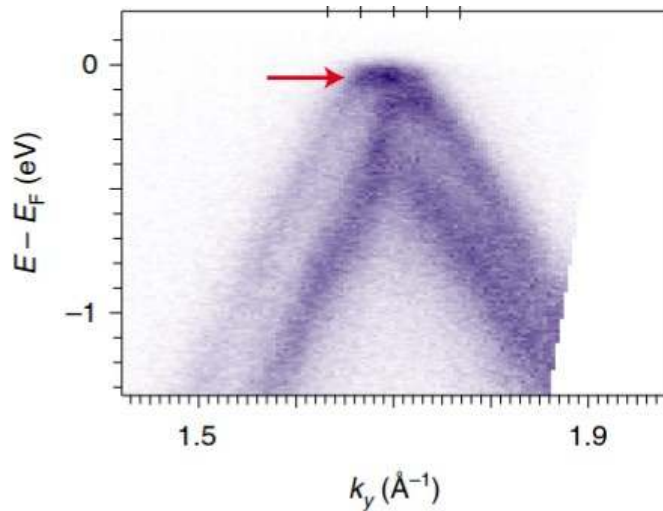
Tiago Antão



arXiv:2512.18397 (2025)

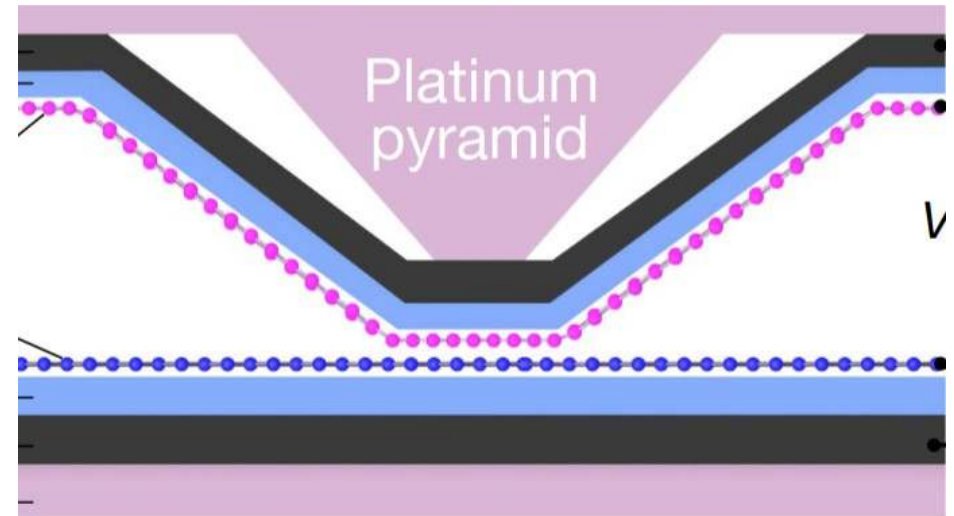
Momentum-resolved spectral functions

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

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

Quantum Fourier transform

Projector in a (large-enough) region

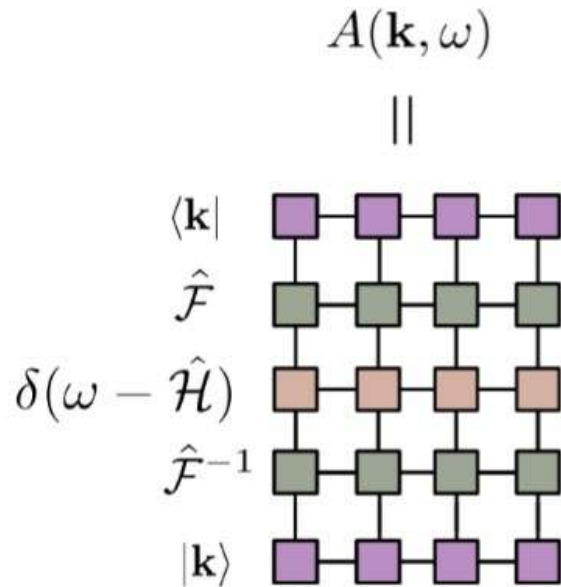
Tensor-network representation of the quantum Fourier transform

$$\begin{aligned} \hat{F} |k\rangle &= \frac{1}{\sqrt{N}} \bigotimes_{r=1}^L \sum_{s_r=0}^1 e^{2\pi i k s_r 2^{-r}} |s_r\rangle \\ &= \bigotimes_{r=1}^L \frac{1}{\sqrt{2}} \left[|0\rangle + e^{2\pi i k 2^{-r}} |1\rangle \right] \end{aligned}$$

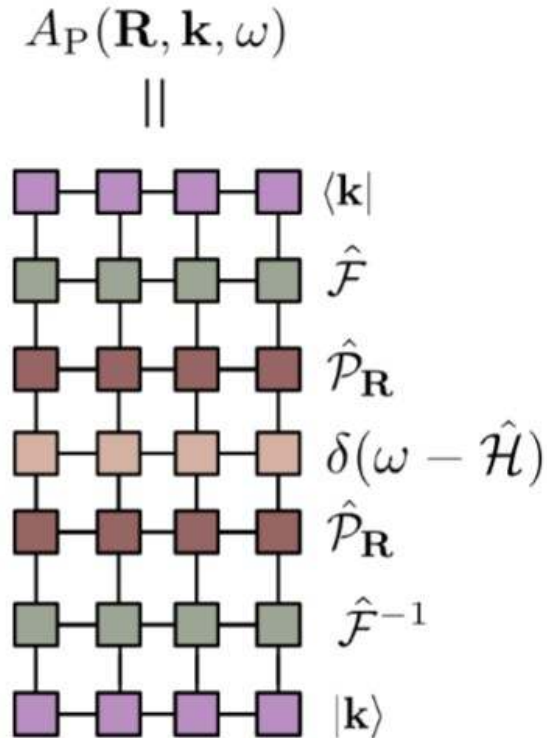


Tensor-network representation of the momentum-resolved spectral function

Total momentum-resolved
spectral function

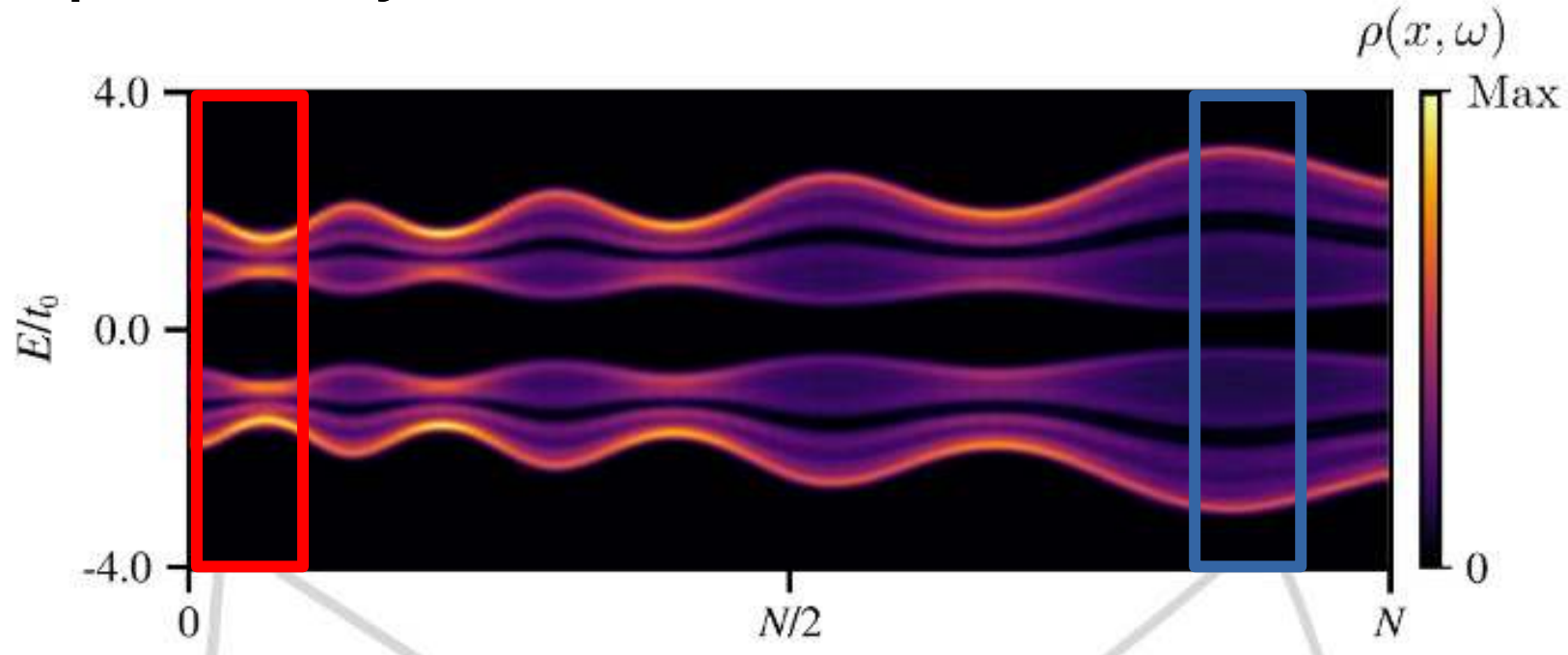


Local momentum-resolved
spectral function



Super-moire with non-uniform strain

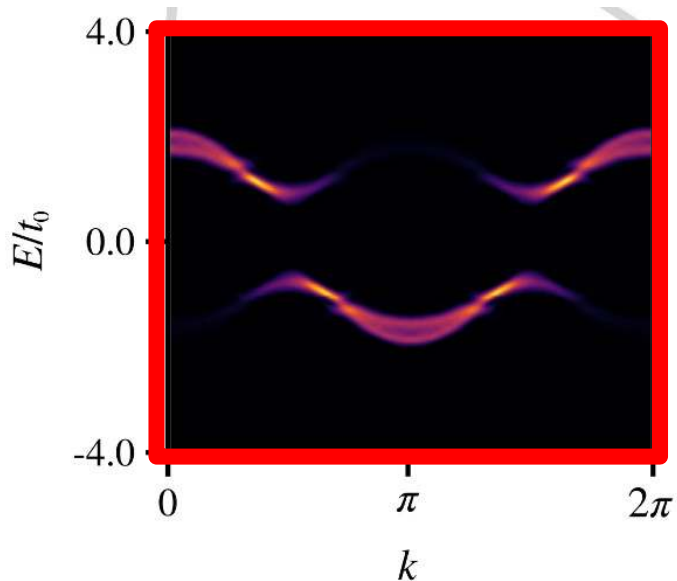
Super-moire system with non-uniform strain and interactions



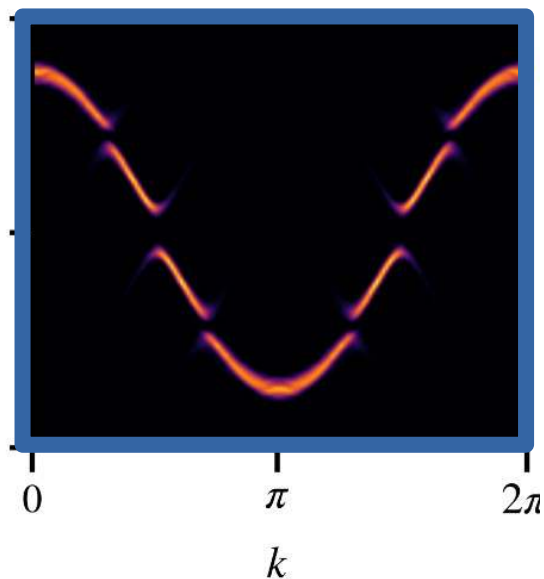
The super-moire features a strongly spatially-dependent electronic structure, that can be imaged in the local momentum-resolved spectral function

Super-moire with non-uniform strain

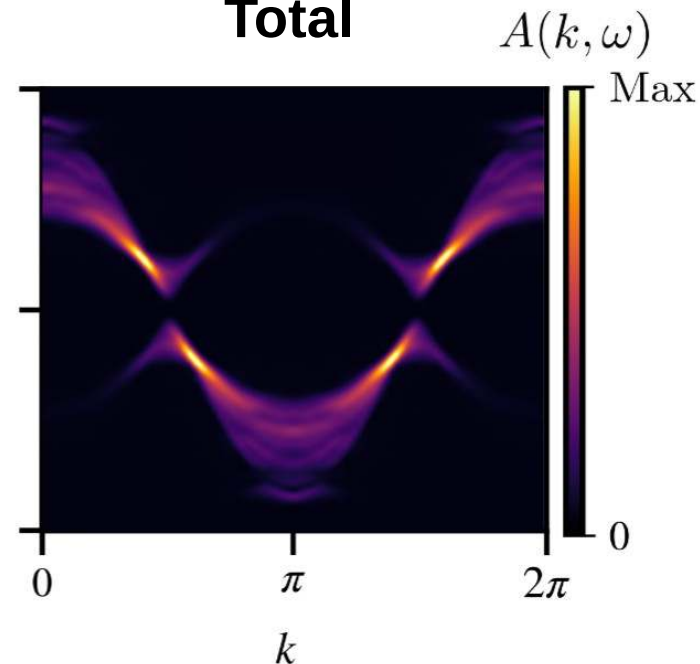
Region #1



Region #2



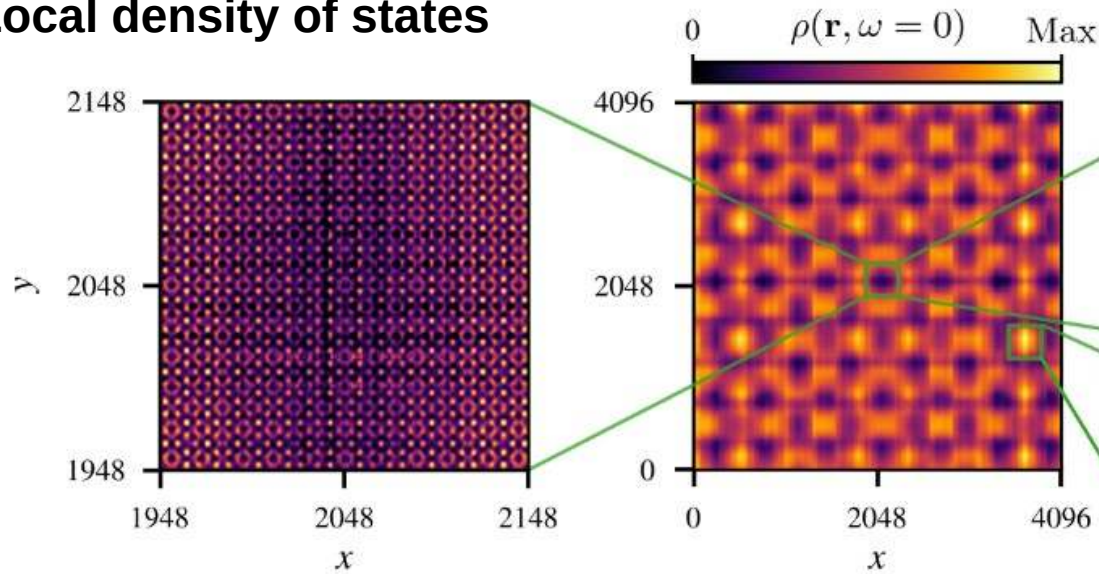
Total



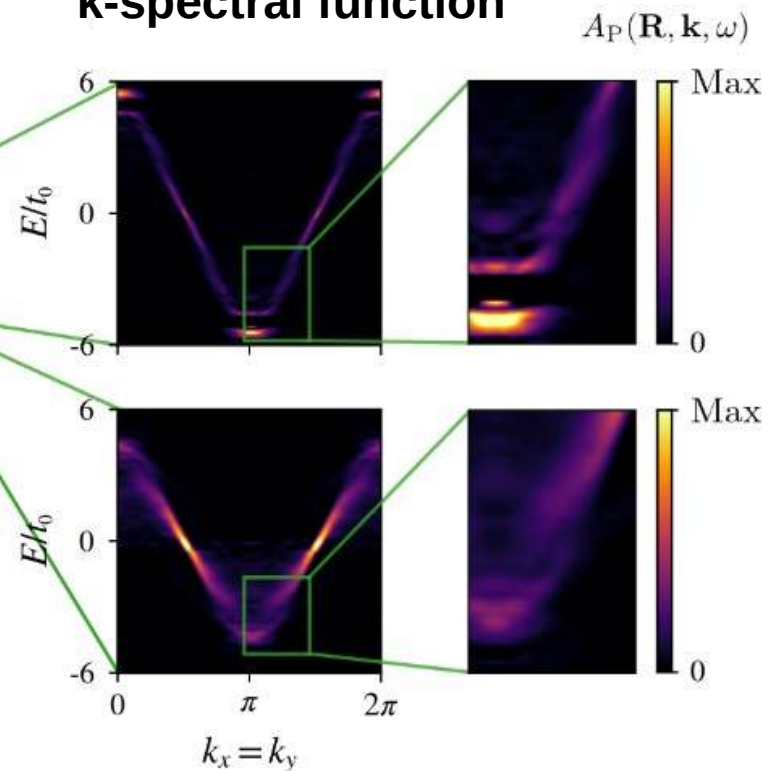
The super-moire features a strongly spatially-dependent electronic structure, that can be imaged in the local momentum-resolved spectral function

8-fold quasicrystal momentum-resolved functions

Local density of states



k-spectral function



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

Future of tensor networks for super-moire

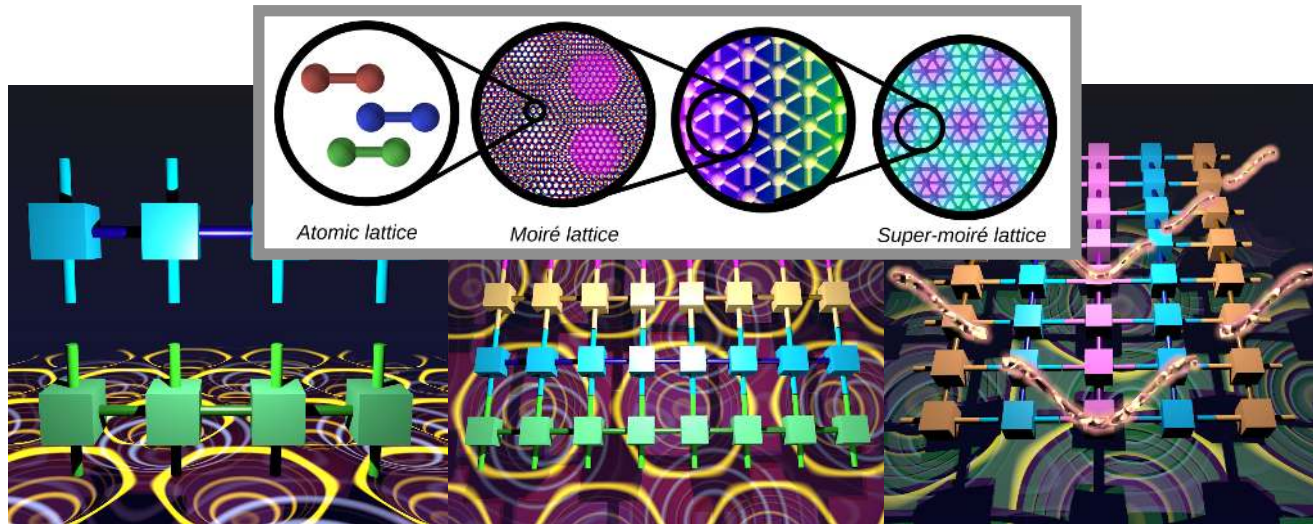
Potential future tensor network methods for super-moire

- 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

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)
arXiv:2506.05230 (2025)
arXiv:2512.18397 (2025)

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