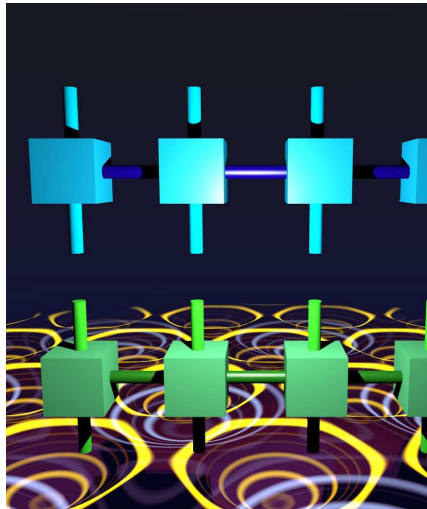
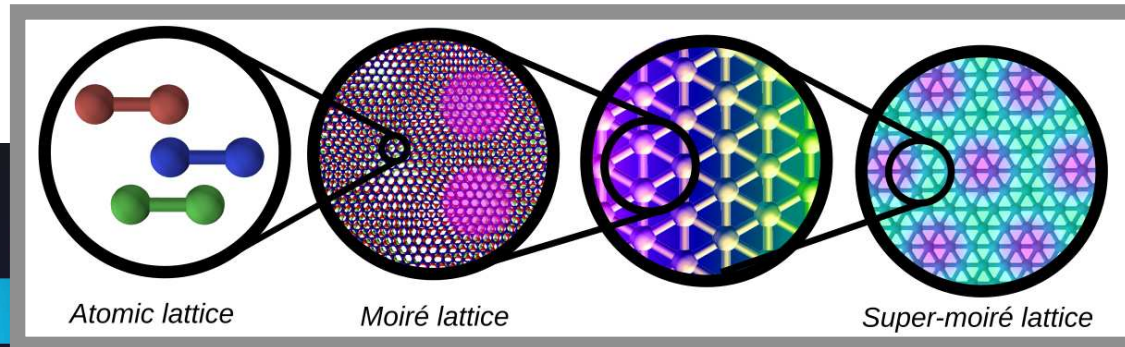


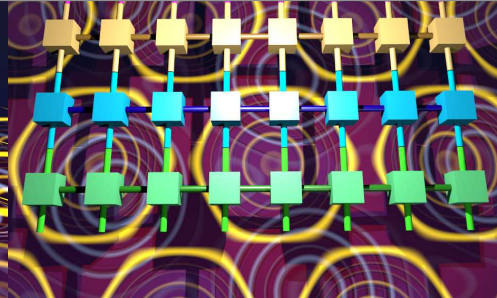
Solving billion-size super-moiré quantum materials with quantum-inspired tensor network algorithms

Jose Lado

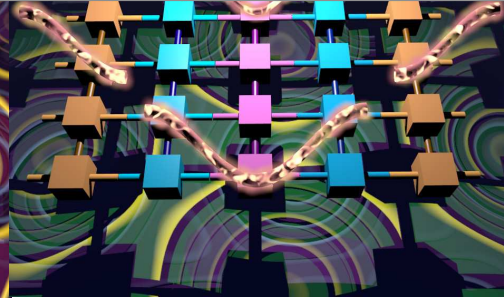
Department of Applied Physics, Aalto University, Finland



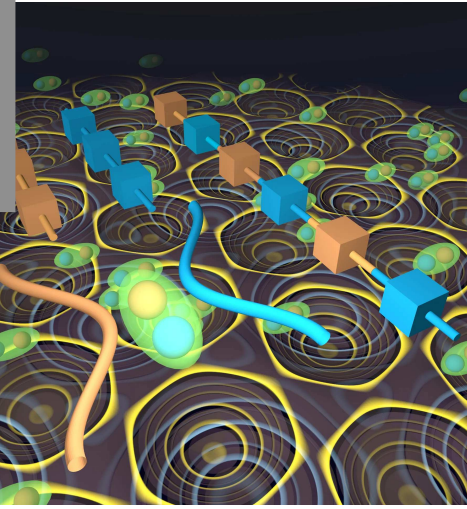
Phys. Rev. Research 7, 043288 (2025)



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



arXiv:2512.18397 (2025)



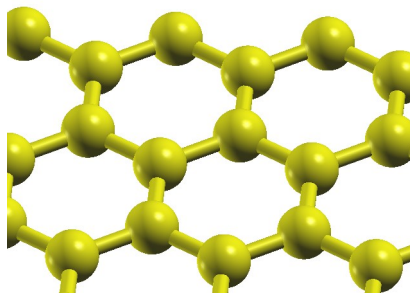
arXiv:2603.02011 (2026)

Quantum Seminar Series, Microsoft Quantum, June 10th 2026

A rich family of electronic orders in 2D materials

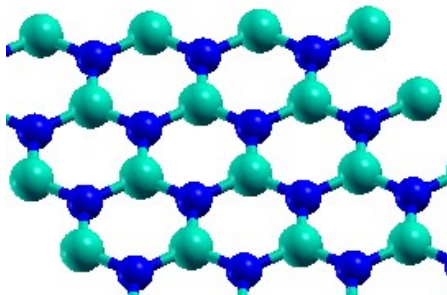
Semimetal

Graphene



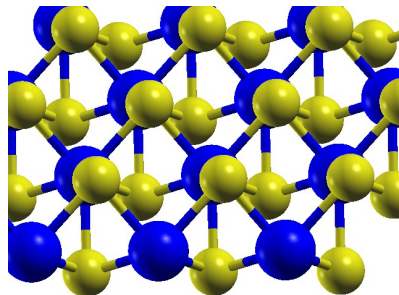
Insulator

BN



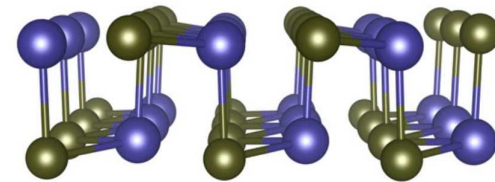
Superconductor

NbSe₂



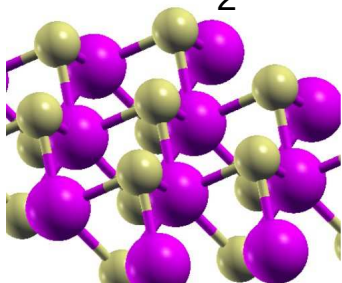
Ferroelectric

SnTe



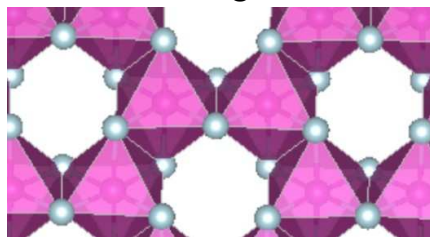
Semiconductor

WS₂



Ferromagnet

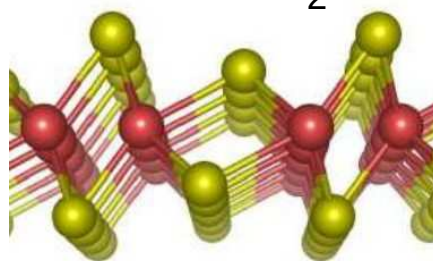
CrI₃



Quantum spin

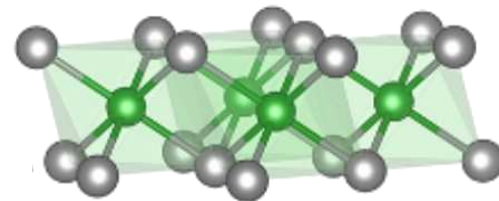
Hall insulator

WTe₂



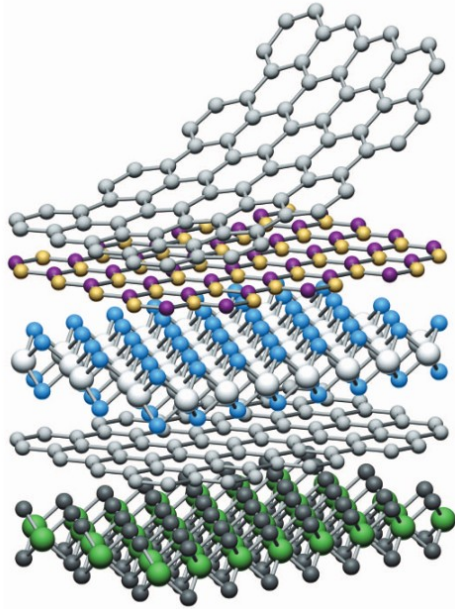
Multiferroic

NiI₂



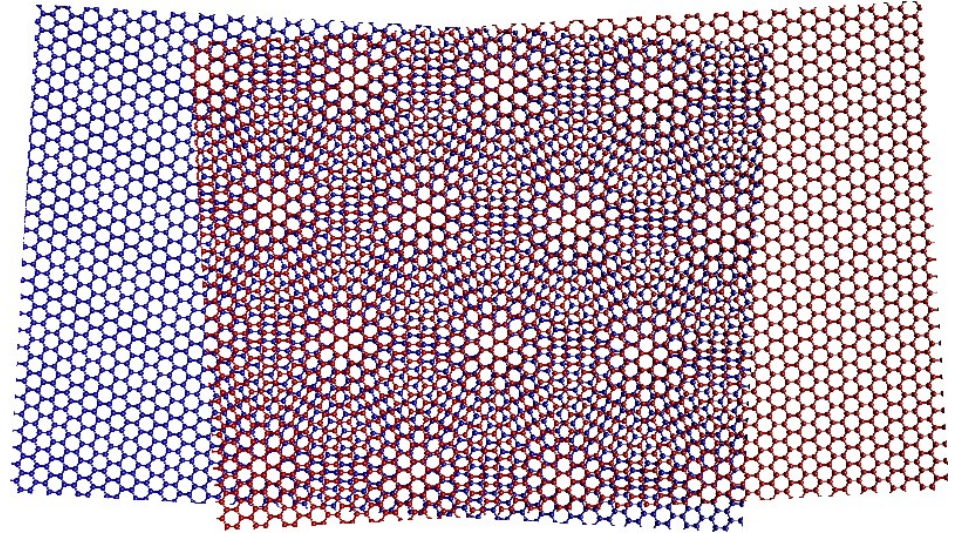
The flexibility of two-dimensional materials

They can be stacked



Nature 499, 419–425 (2013)

They can be rotated

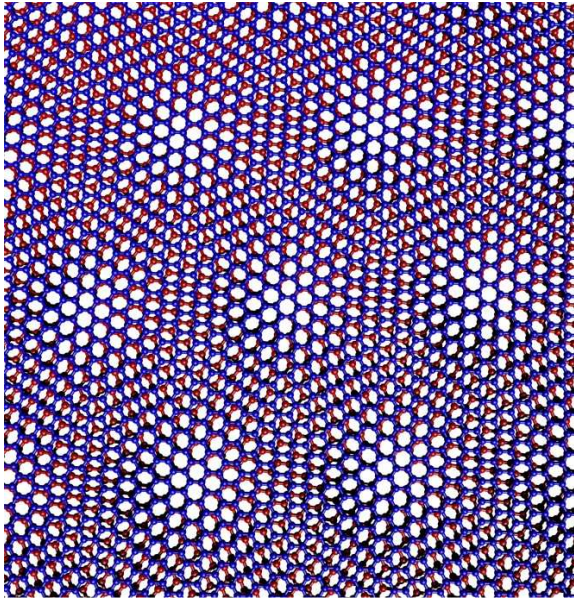


Science 361, 6403, 690-693 (2018)

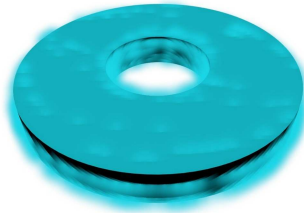
These are unique features of two-dimensional materials

The tunability of twisted van der Waals materials

Twisted bilayer graphene

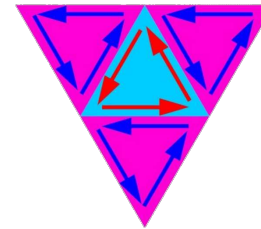


Superconductivity



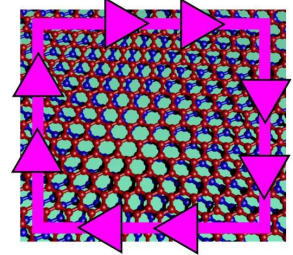
Nature 556, 43–50 (2018)

Topological networks



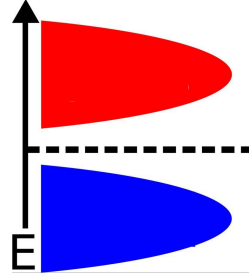
Nano Lett. 18, 11, 6725-6730 (2018)

Chern insulators



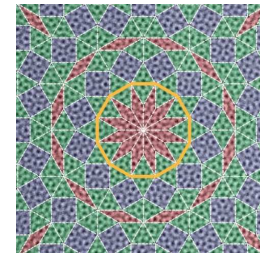
Science 365, 605-608 (2019)

Correlated insulators



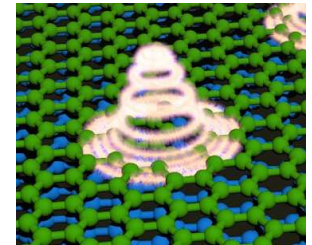
Nature 556, 80–84 (2018)

Quasicrystalline physics



Science 361, 782-786 (2018)

Proximal fractional Chern insulators

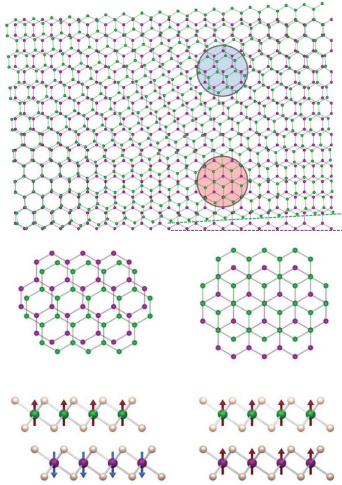


Nature 600, 439–443 (2021)

Twisted multilayers provide a powerful platform for emergent phenomena

Artificial quantum matter in moire van der Waals heterostructures

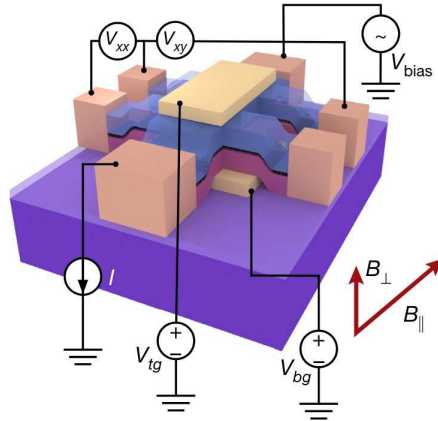
Unconventional magnets



Twisted CrBr_3

Science, 374(6571),
1140–1144 (2021)

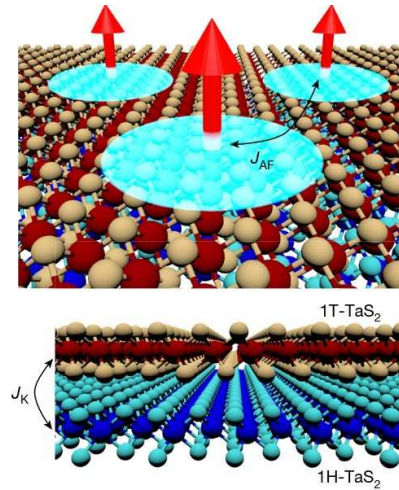
Unconventional superconductors



Twisted trilayer
graphene

Nature 595,
526–531 (2021)

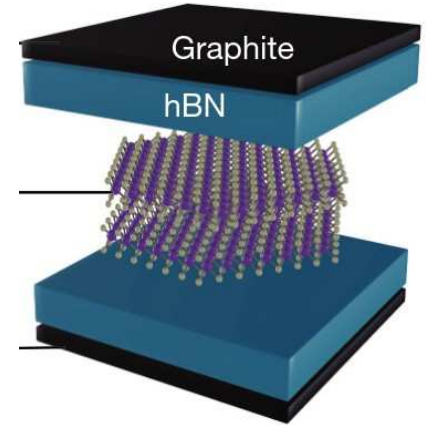
Heavy-fermion quantum materials



1H-1T TaS_2

Nature 599,
582–586 (2021)

Fractional topological matter

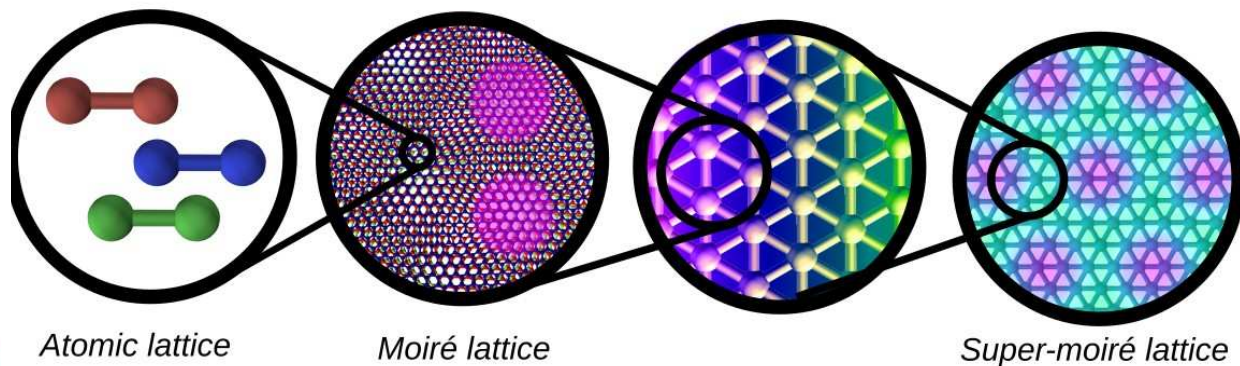
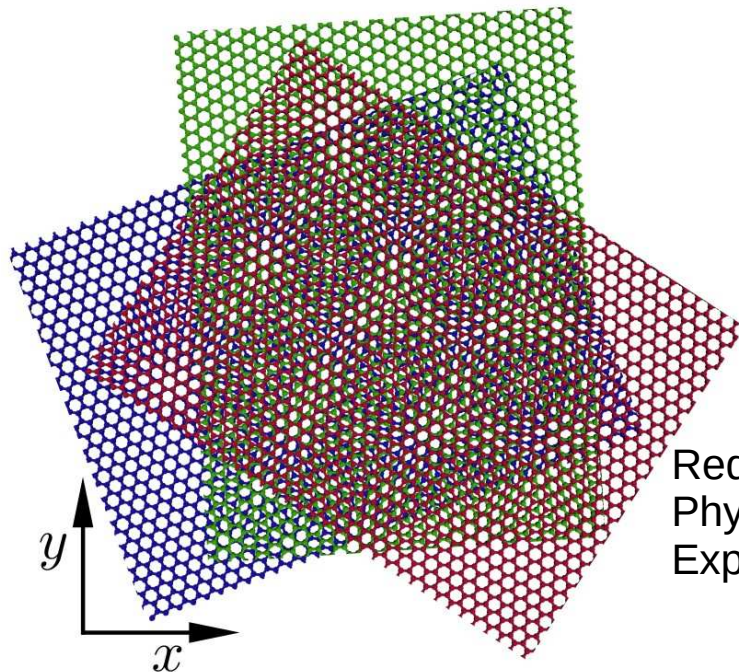


Twisted MoTe_2

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

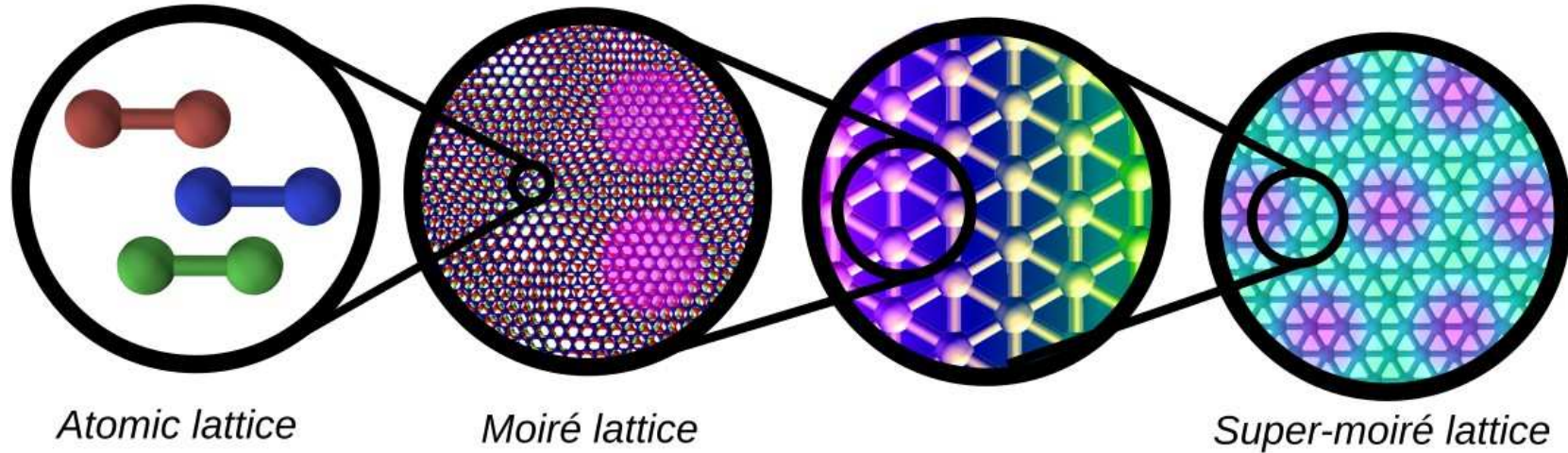
Nature 620, 762–767 (2023)

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)

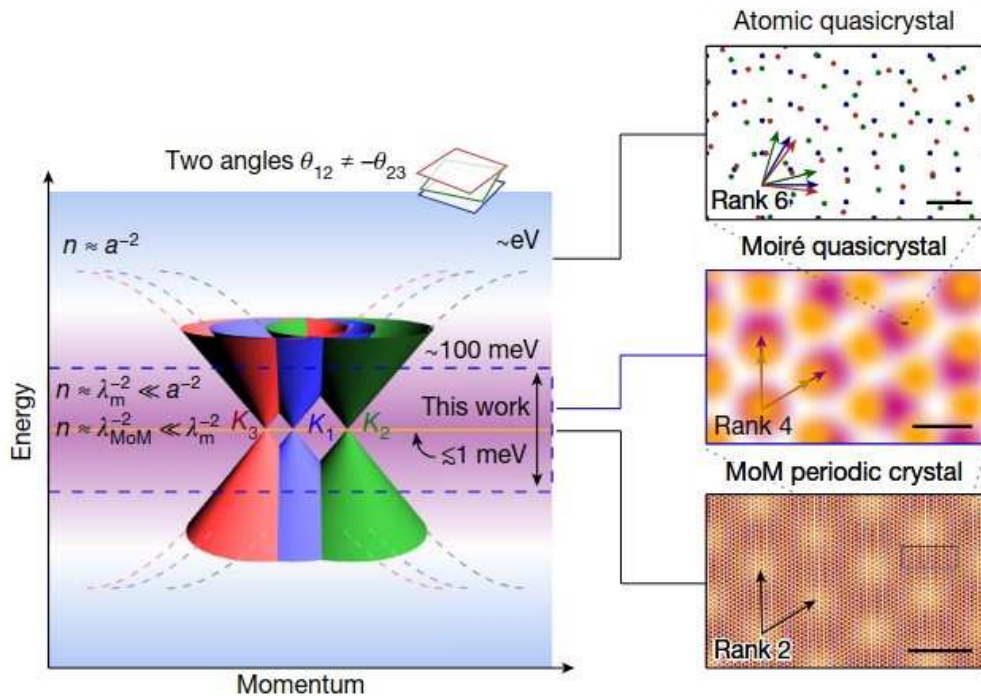
Super-moiré **$N=10^9$ sites**, calculations taking 10 days – 1000000 years

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

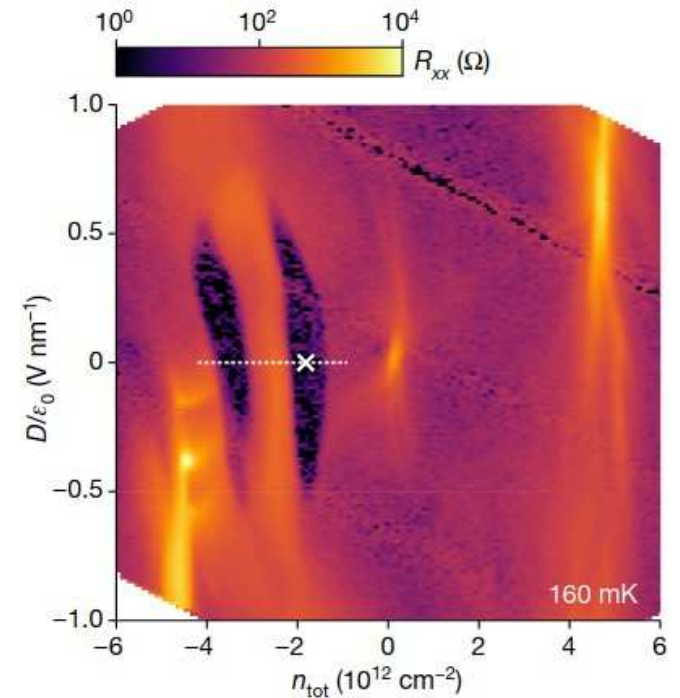
(even going beyond usual memory limitations of conventional methods)

Super-moire materials, experimentally

Moire quasicrystal in twisted trilayer graphene



Coexisting correlations and superconductivity



Behind the scenes

Yitao Sun



Tiago Antão



Anouar Moustaj



Lumen Eek



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)

Tensor-network methodology for super-moiré excitons beyond one billion sites, A. Moustaj, Y. Sun, T. V. C. Antão, L. Eek, J. L. Lado, **arXiv:2603.02011** (2026)

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

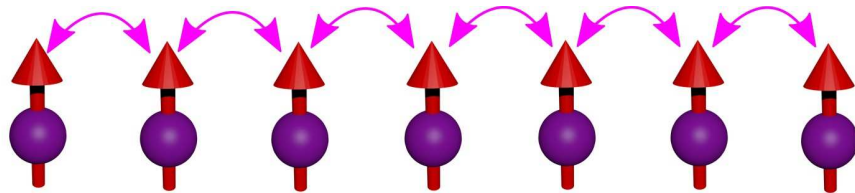
The problem of dimensionality

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

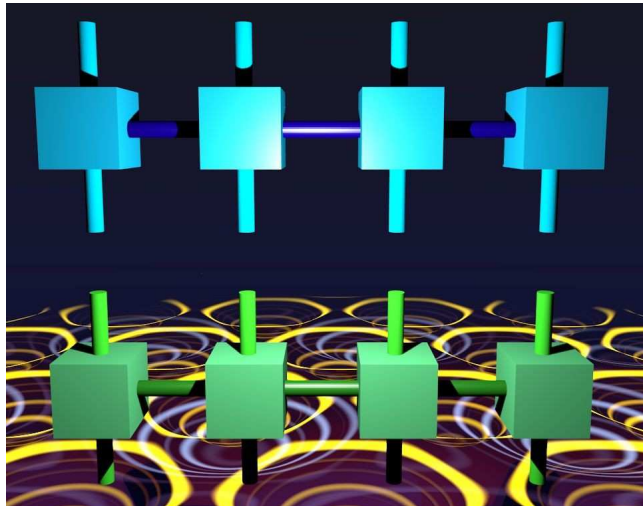
Is there an efficient way of storing so many coefficients?

Dealing with very large spaces with tensor networks

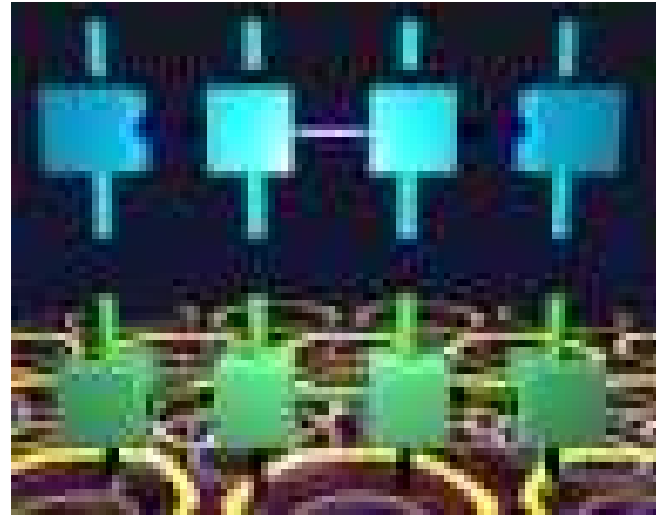
A many-body wavefunction is a very high dimensional object (2^L coefficients)

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

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



“True wavefunction”



“Tensor-network wavefunction”

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

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



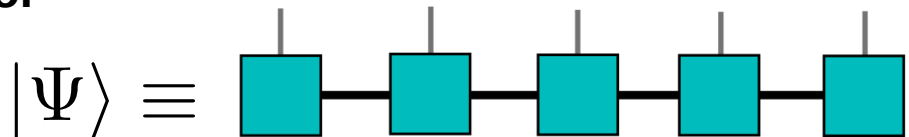
Matrix product state

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

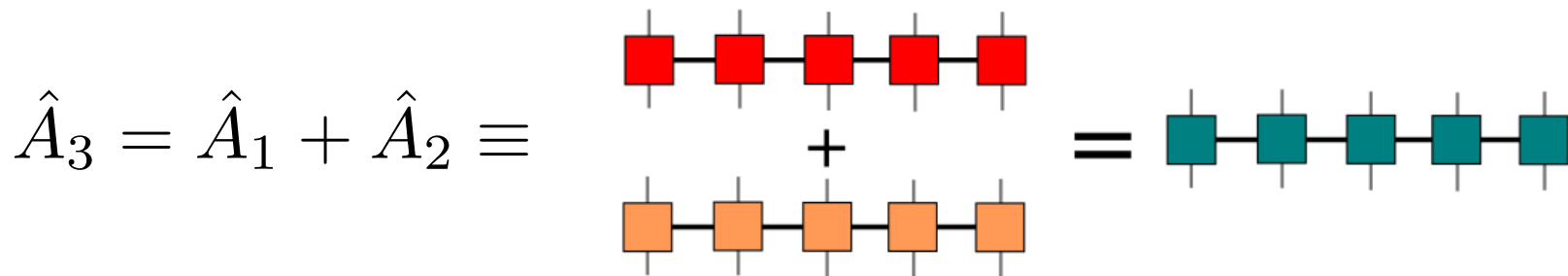
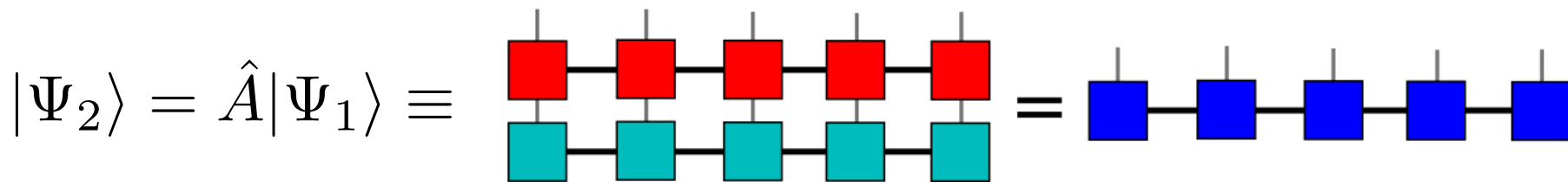
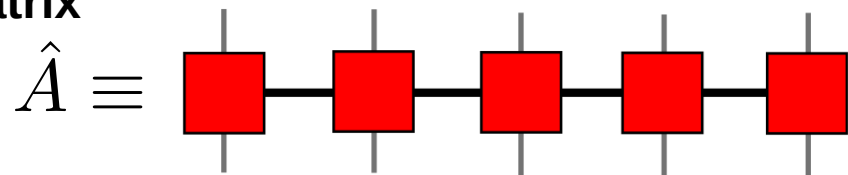
Exponentially large algebra with tensor networks

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

vector



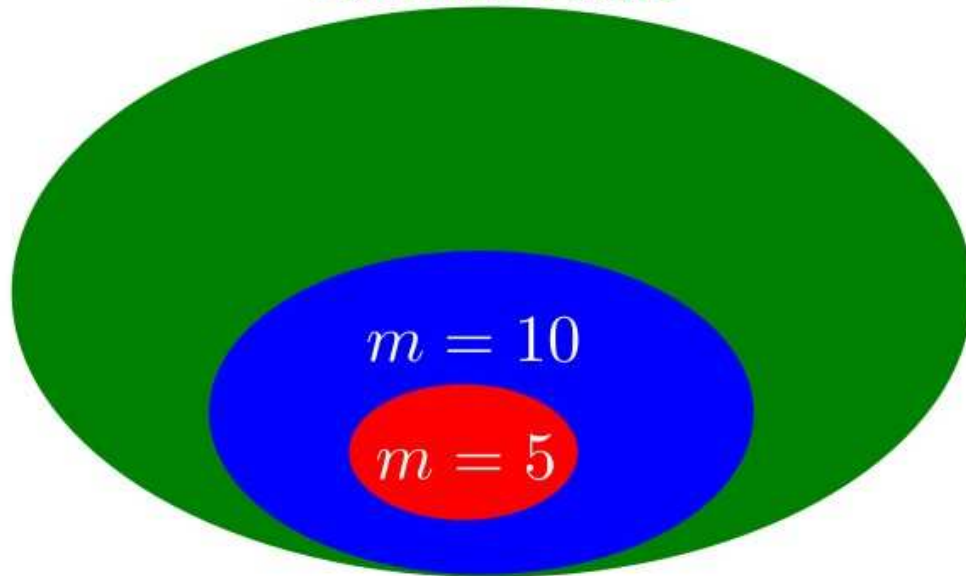
matrix



MPS as a parametrization of finite entanglement states

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

Full Hilbert state



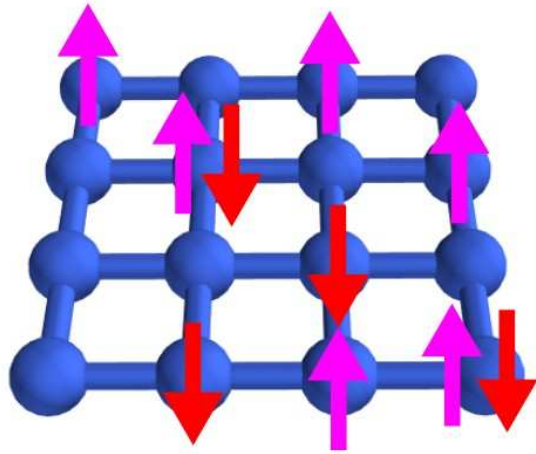
Tensor network states

MPS have an entanglement entropy
bounded by the bond dimension

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

Some paradigmatic problems solved with matrix product states

Solving the 2D Hubbard model at finite doping

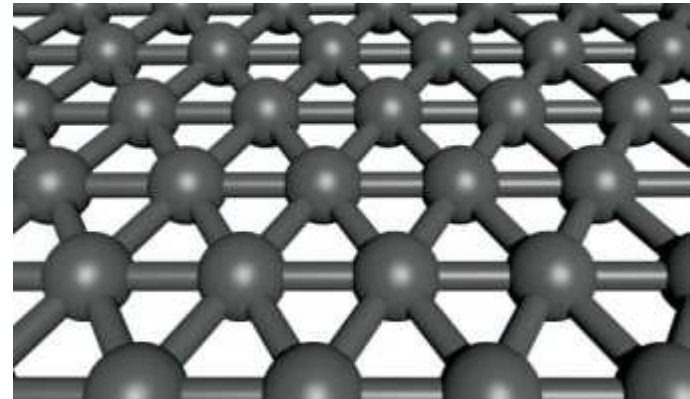


$$H = \sum_{ij,s} t_{ij} c_{is}^\dagger c_{js} + \sum_i U c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow}$$

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

Science, 384(6696), eadh7691 (2024)

Solving the 2D Heisenberg model in frustrated lattices



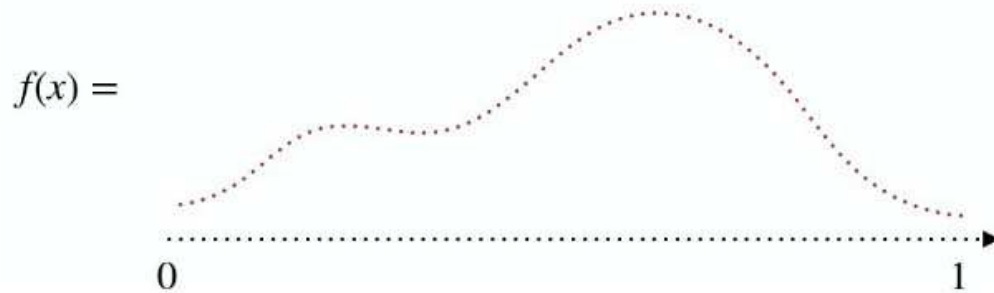
$$\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

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

Phys. Rev. X 10, 021042 (2020)

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

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

[illegible]

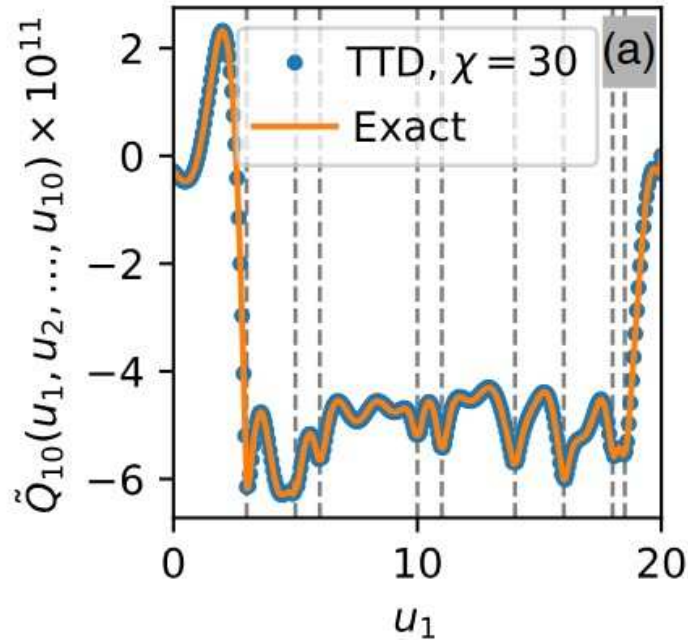
Quantum inspired active learning to learn exponentially large spaces

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

SciPost Phys. 18, 104 (2025)

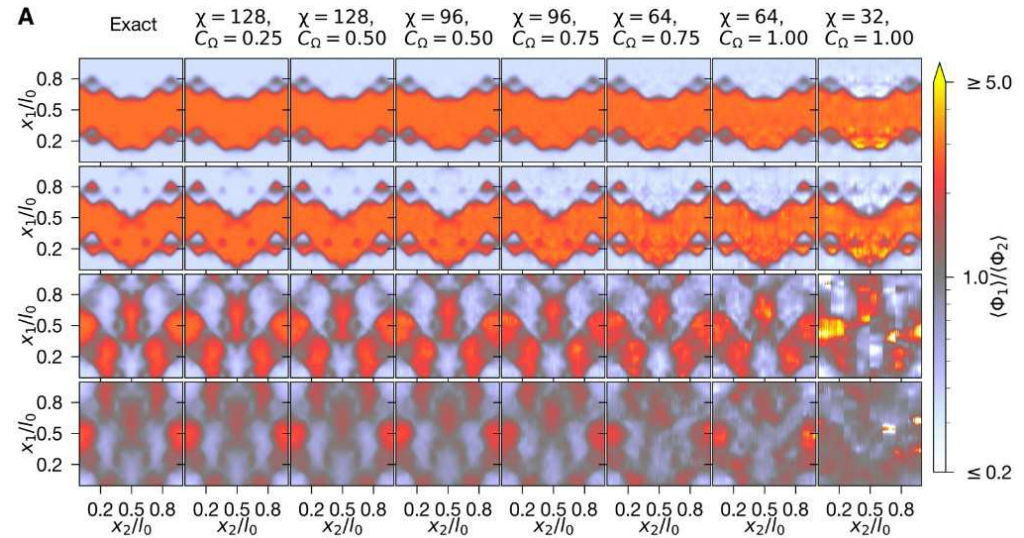
Learning exponentially large spaces with tensor networks

High dimensional integrals for Feynman diagrams



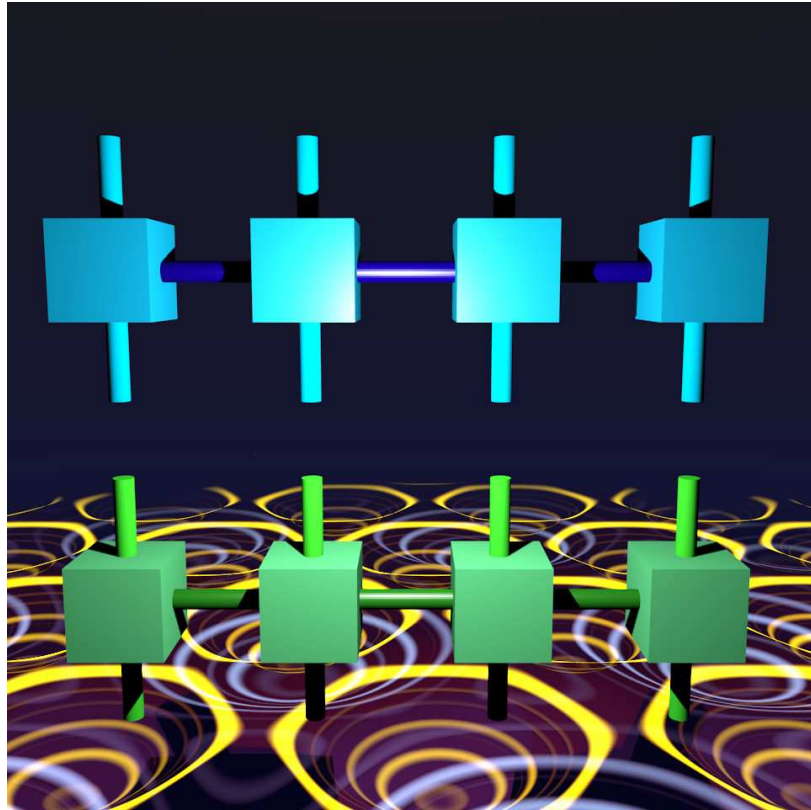
Phys. Rev. X 12, 041018 (2022)

Probabilistic turbulence distributions



Science Advances, 11(5), eads5990 (2025)

Tensor-networks for interacting super-moire materials



Phys. Rev. Research 7, 043288 (2025)

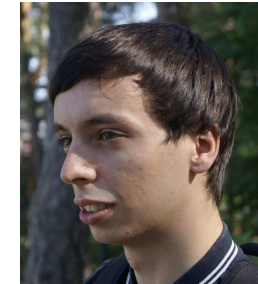
Yitao Sun



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

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

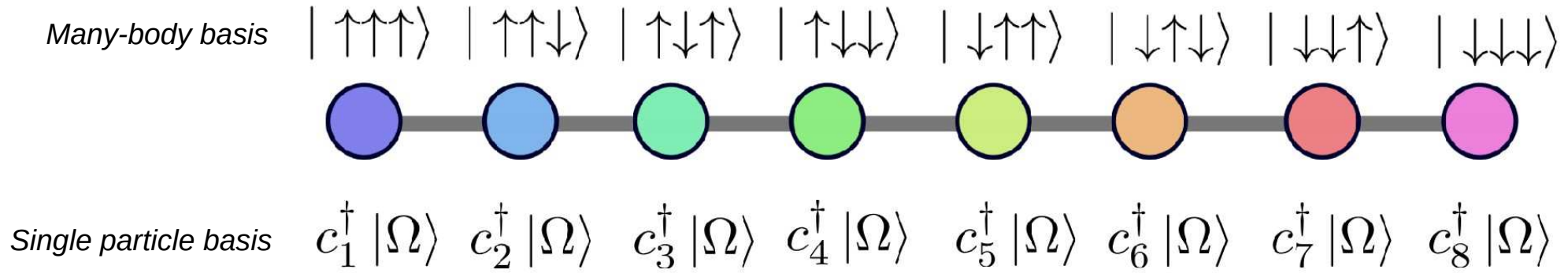
Solving the system requires dealing with matrices proportional to the system size

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

$$\mathcal{H}_{\alpha\beta}^{MF} \equiv \Gamma_{s_1, s'_1}^{(1)} \Gamma_{s_2, s'_2}^{(2)} \Gamma_{s_3, s'_3}^{(3)} \dots \Gamma_{s_L, s'_L}^{(L)}$$

$$\mathcal{H}_{\alpha\beta}^{MF} \equiv \text{[Diagram: A sequence of orange squares connected horizontally, representing a tensor network.]}$$

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

Tensor Network SCF loop

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

Kernel polynomial tensor network algorithm

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

$$\hat{\mathcal{P}} = \int_{-\infty}^{\epsilon_F} \delta(\omega - \hat{H}) d\omega \equiv \begin{array}{c} | \\ \text{---} \square \text{---} \square \text{---} \dots \text{---} \square \text{---} \\ | \end{array}$$

With a kernel polynomial tensor network algorithm

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

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

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

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

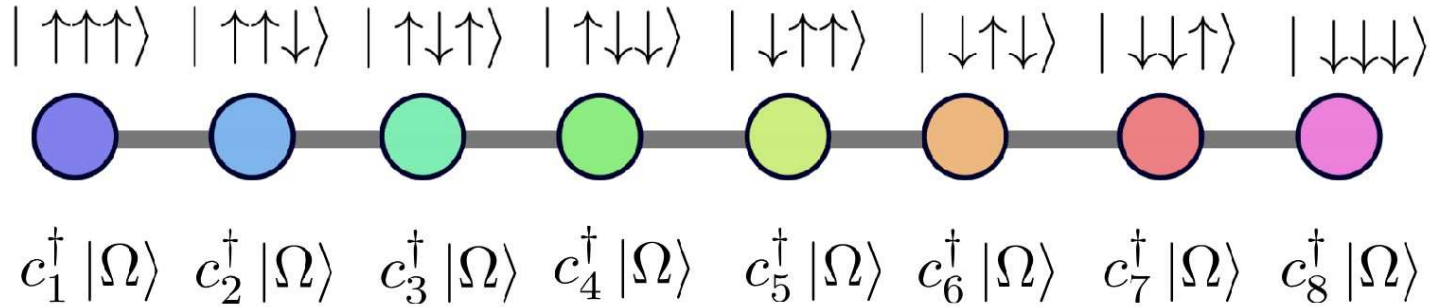
$$P_n(\omega) = \frac{2T_n(\omega)}{\pi\sqrt{1-\omega^2}}$$

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

$$\mathcal{H}_{\alpha\beta}^{MF} \equiv \text{[Tensor Network Diagram]}$$

Tensor network representation of a super-movie Hamiltonian

Let us start with a uniform hopping Hamiltonian



In the tight binding basis uniform hopping takes the form

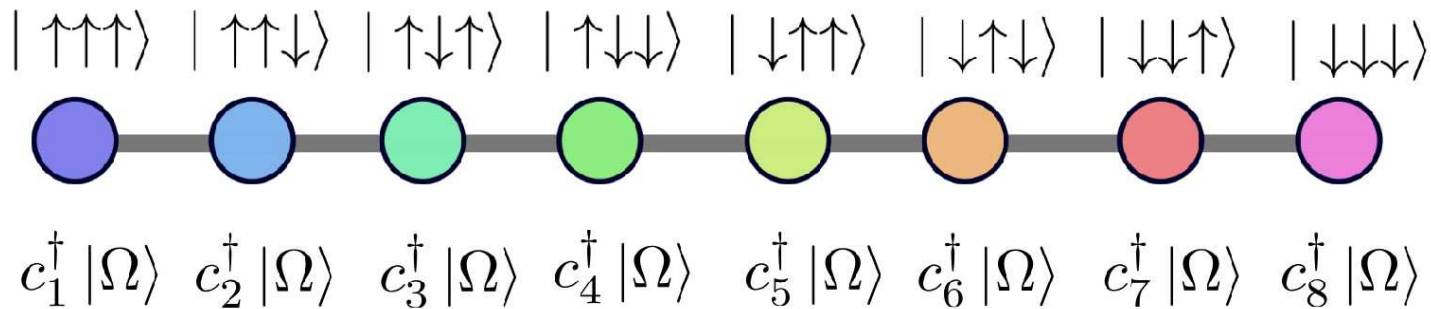
$$H_{0,NN} = \sum_{\alpha,s}^{N-1} t(c_{x_{\alpha+1},s}^\dagger c_{x_{\alpha},s} + h.c.)$$

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

Let us now consider a modulated hopping Hamiltonian



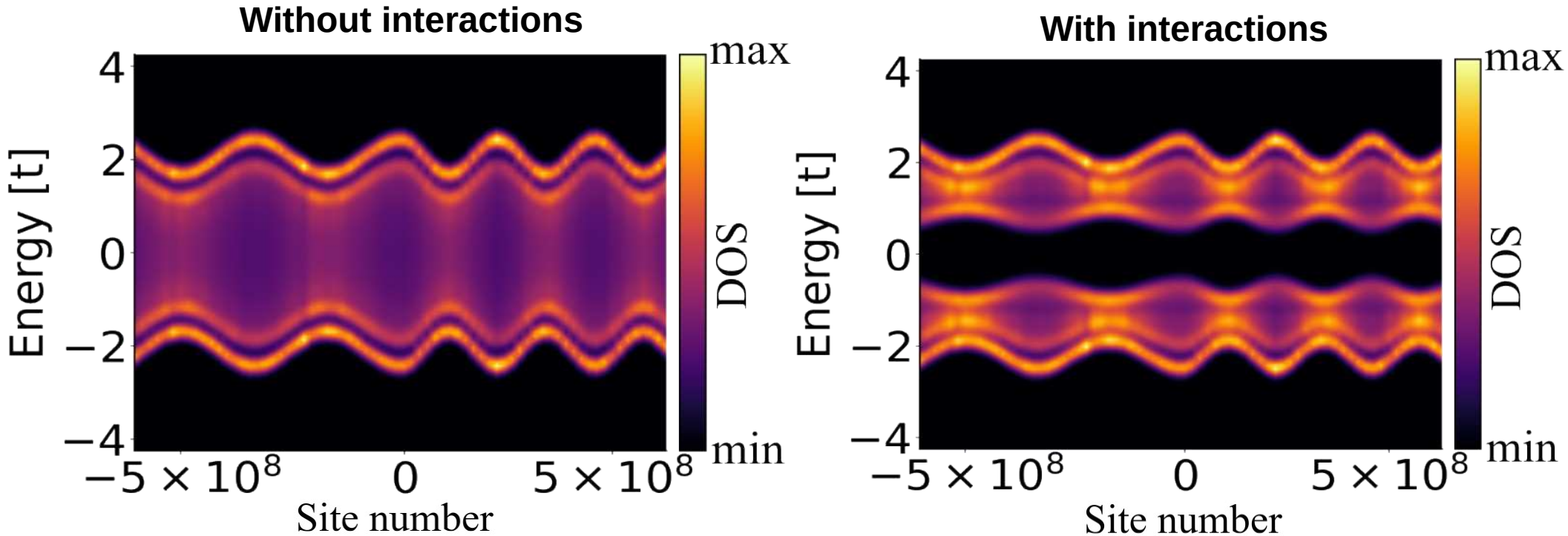
Find the MPS representation for the modulation and store in a diagonal MPO $\mathcal{T}$

$$|\tau\rangle = \sum M_{s_1}^{(1)} M_{s_2}^{(2)} M_{s_3}^{(3)} \dots M_{s_L}^{(L)} |s_1, s_2, \dots, s_L\rangle \quad \text{Quantics tensor cross interpolation}$$

Modulated super-moire by contraction

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

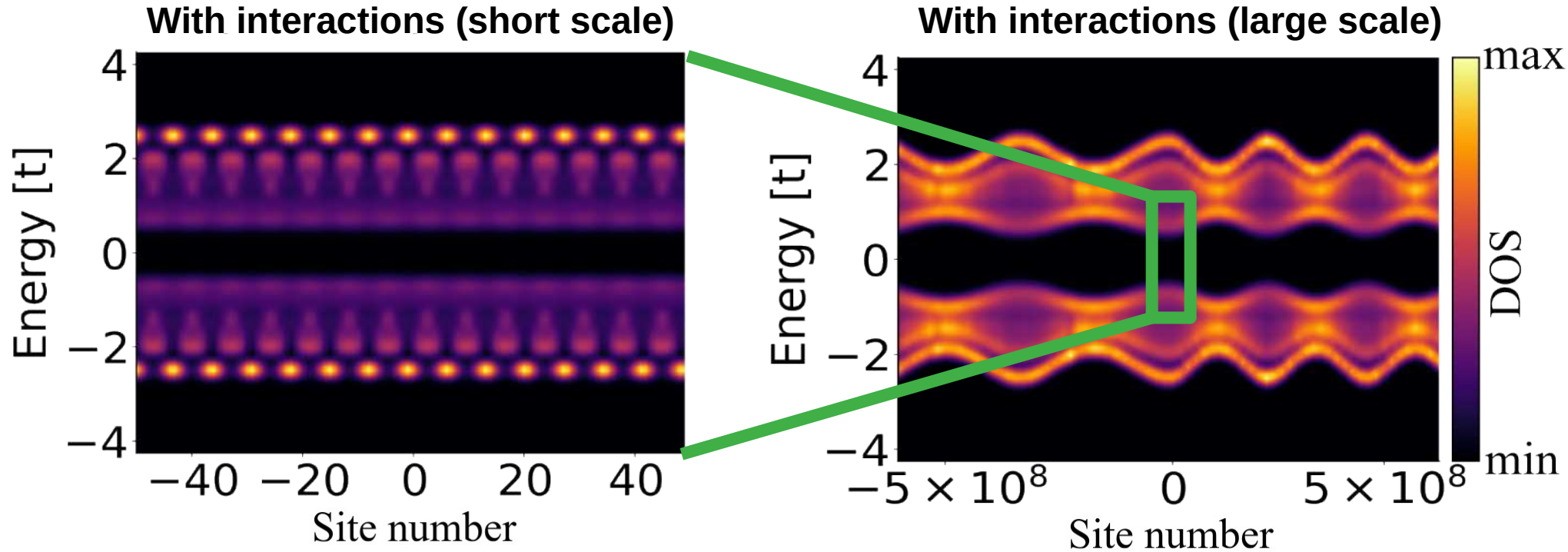
Solving billion-size super-moire materials



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

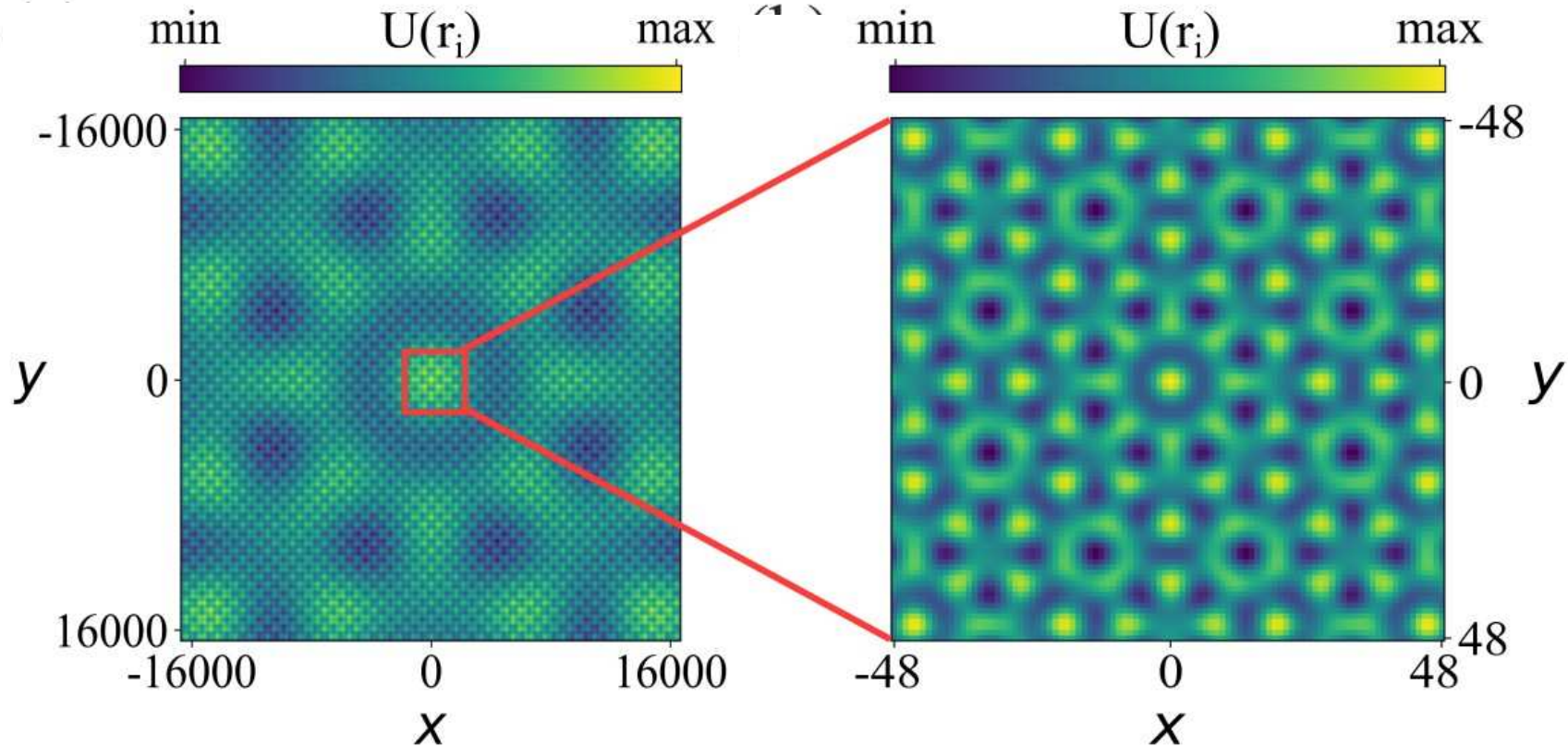


Tensor networks allow to solve selfconsistently a super-moire with one billion sites

Phys. Rev. Research 7, 043288 (2025)

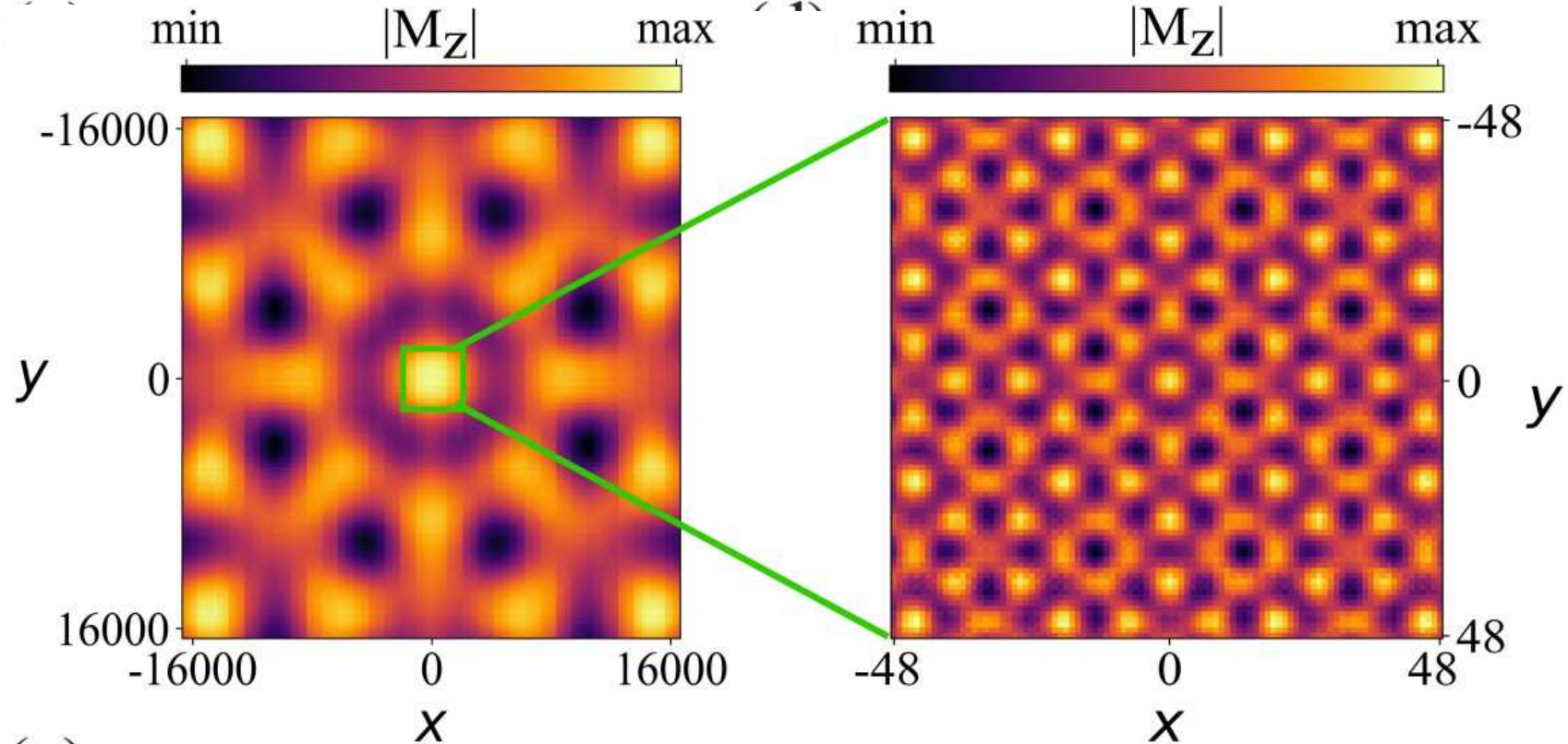
Two-dimensional billion size interacting super-moire

Modulation to the Hamiltonian



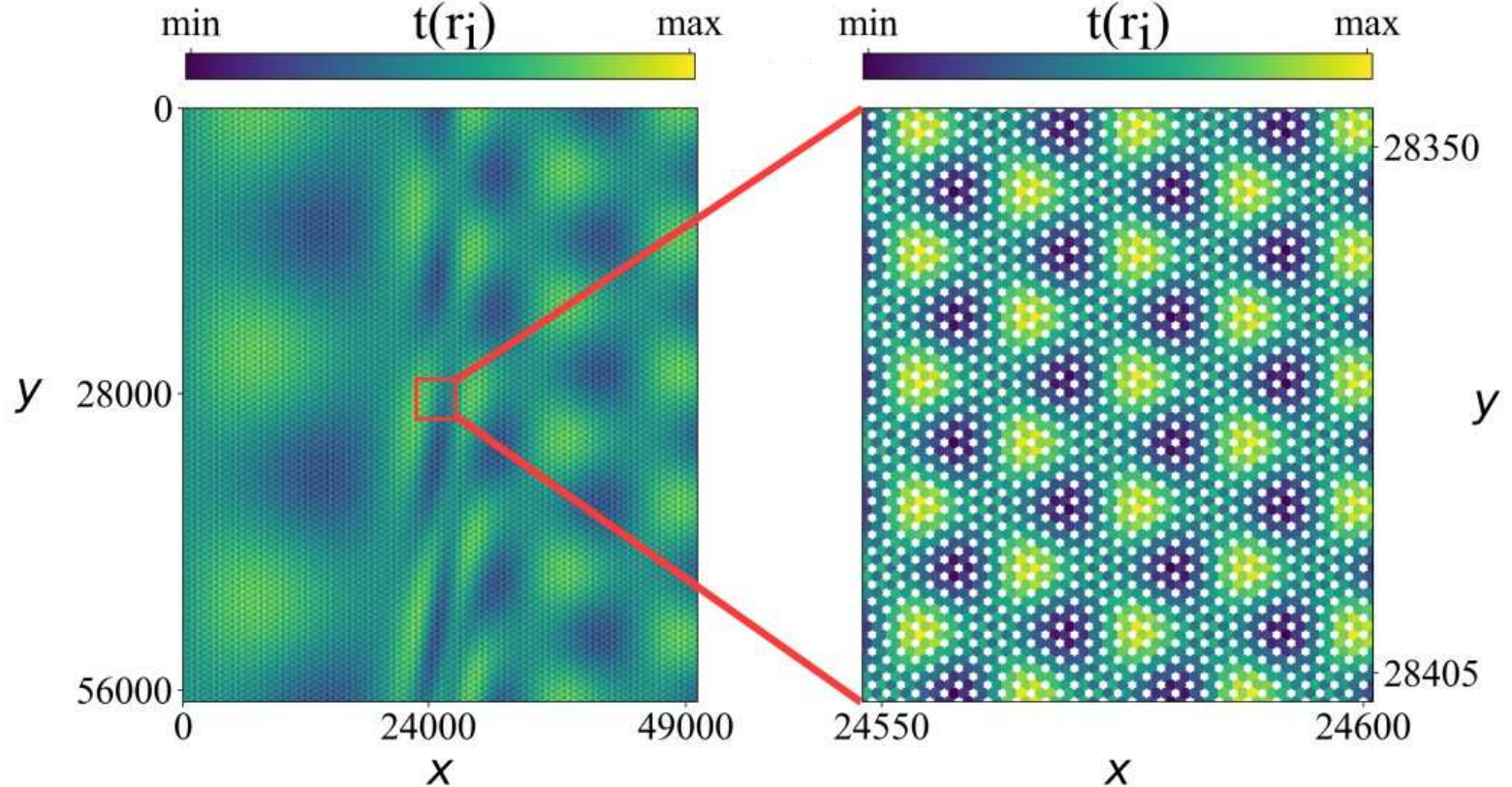
Two-dimensional billion size interacting super-moire

Selfconsistent symmetry broken order (magnetization)



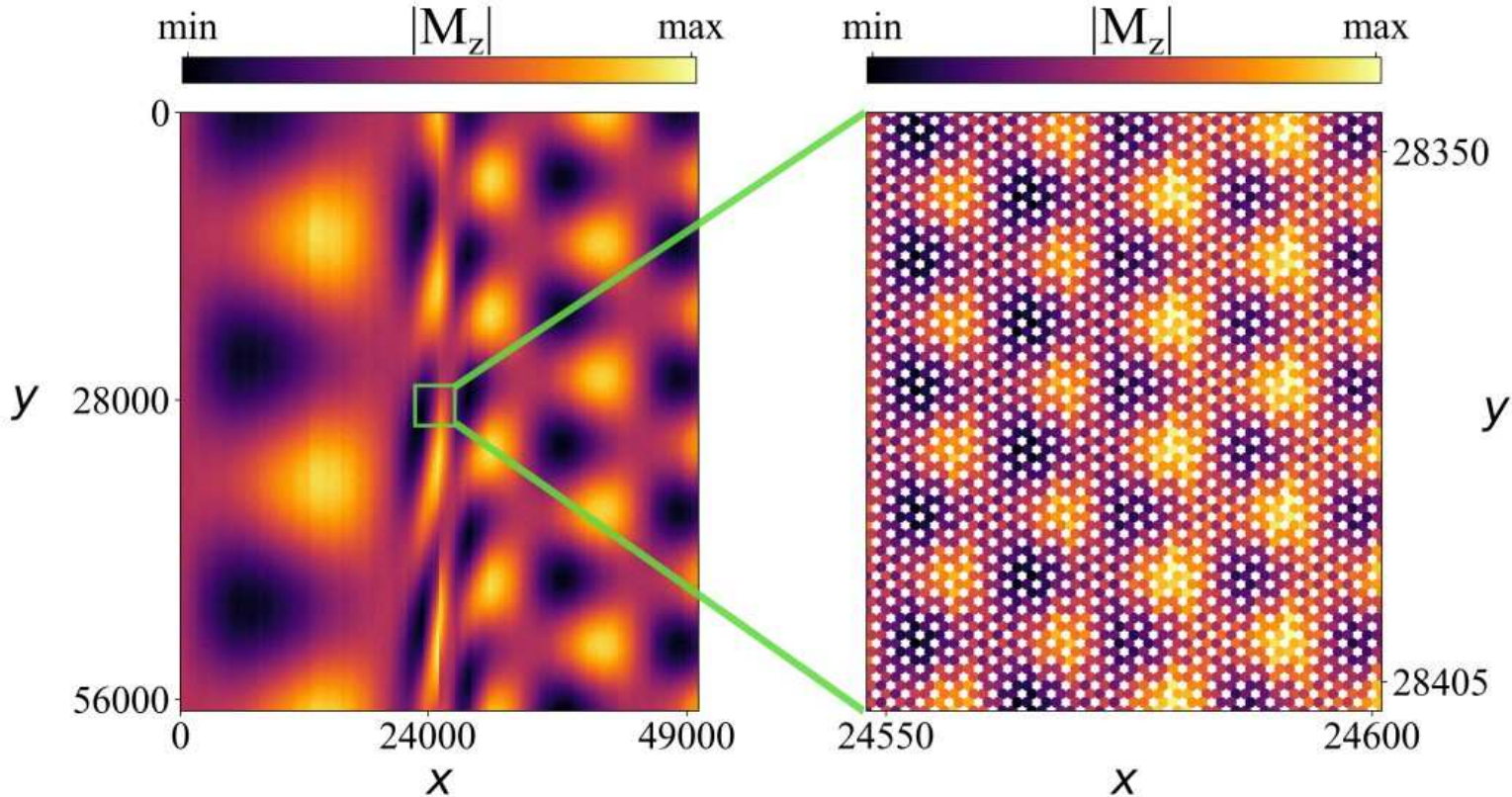
Two-dimensional billion size interacting super-moire

Modulation fo the Hamiltonian

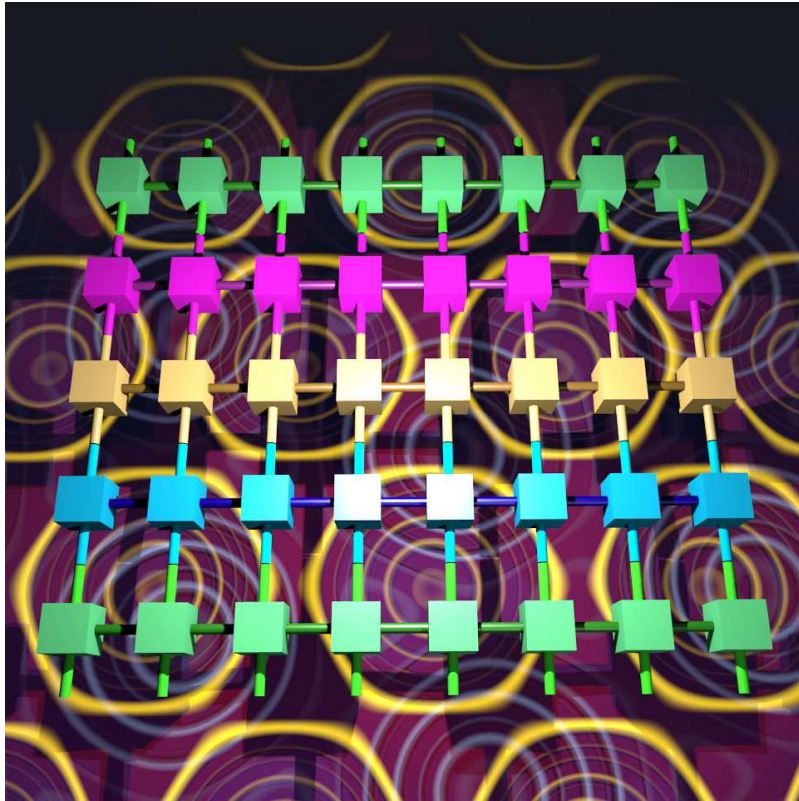


Two-dimensional billion size interacting super-moire

Selfconsistent symmetry broken order (magnetization)



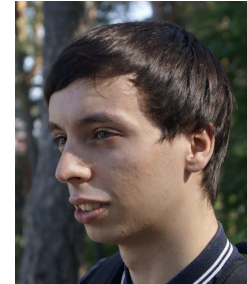
Tensor networks for topological super-moire materials



Yitao Sun



Tiago Antão

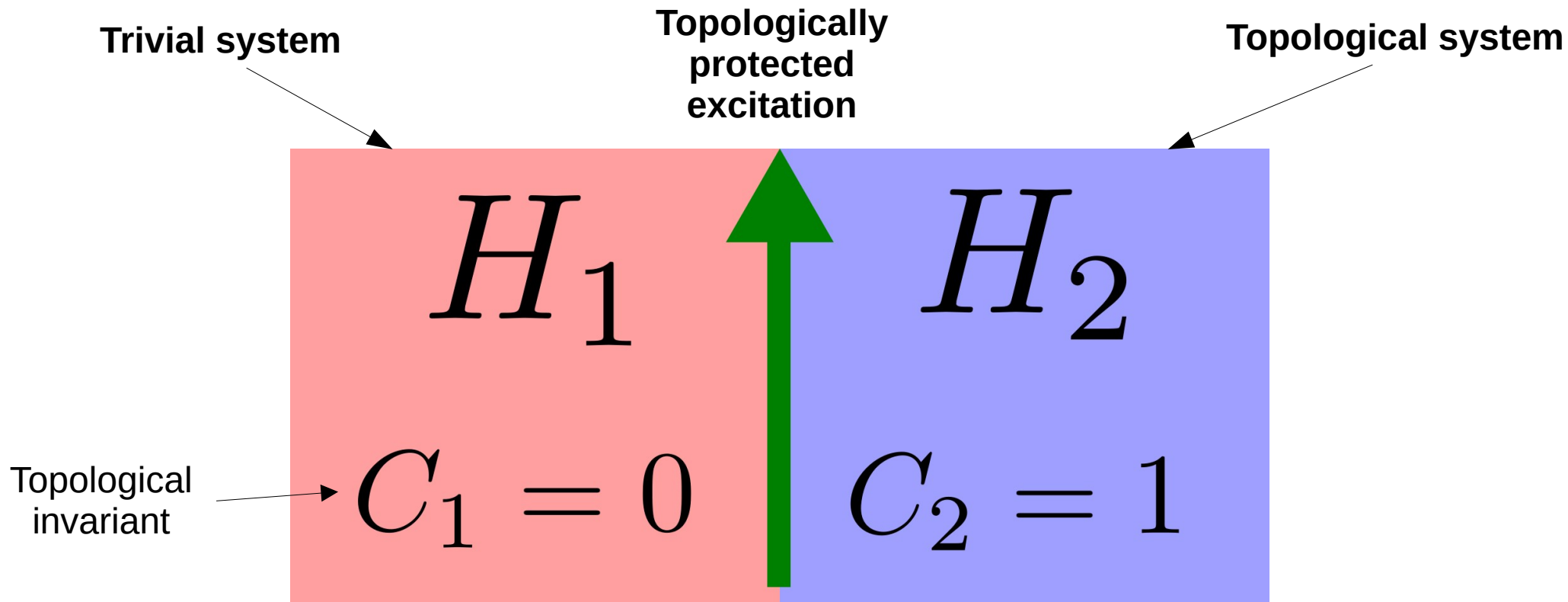


Adolfo
Fumega



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

Topological states and edge modes



Topological excitations appear between topologically different systems

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)

$$A_{\mu}^{\alpha} = i\langle \partial_{k_{\mu}} \Psi_{\alpha} | \Psi_{\alpha} \rangle$$
$$\Omega = \nabla \times \mathbf{A}|_z$$

Metric
(Berry curvature)

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

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

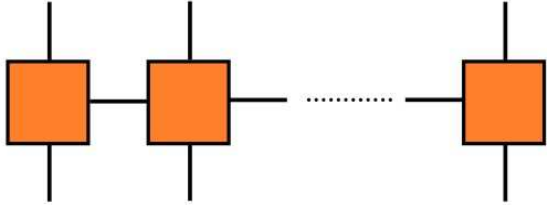
With a kernel polynomial tensor network algorithm

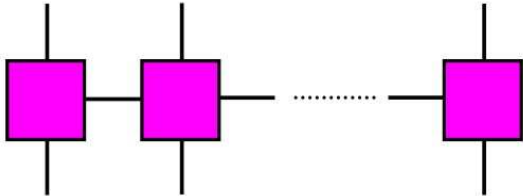
$$\hat{\mathcal{P}} = \sum_n T_n(\hat{\mathcal{H}}) \int_{-\infty}^{\varepsilon_F} d\omega \frac{T_n(\omega)}{\sqrt{1 - \omega^2}},$$

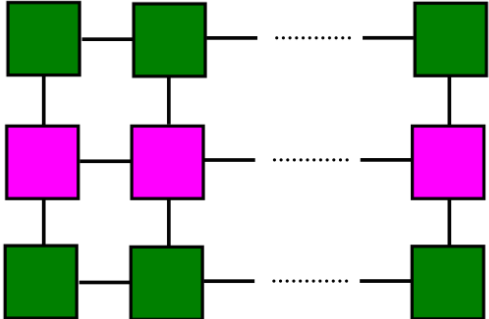
$$T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x)$$

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

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

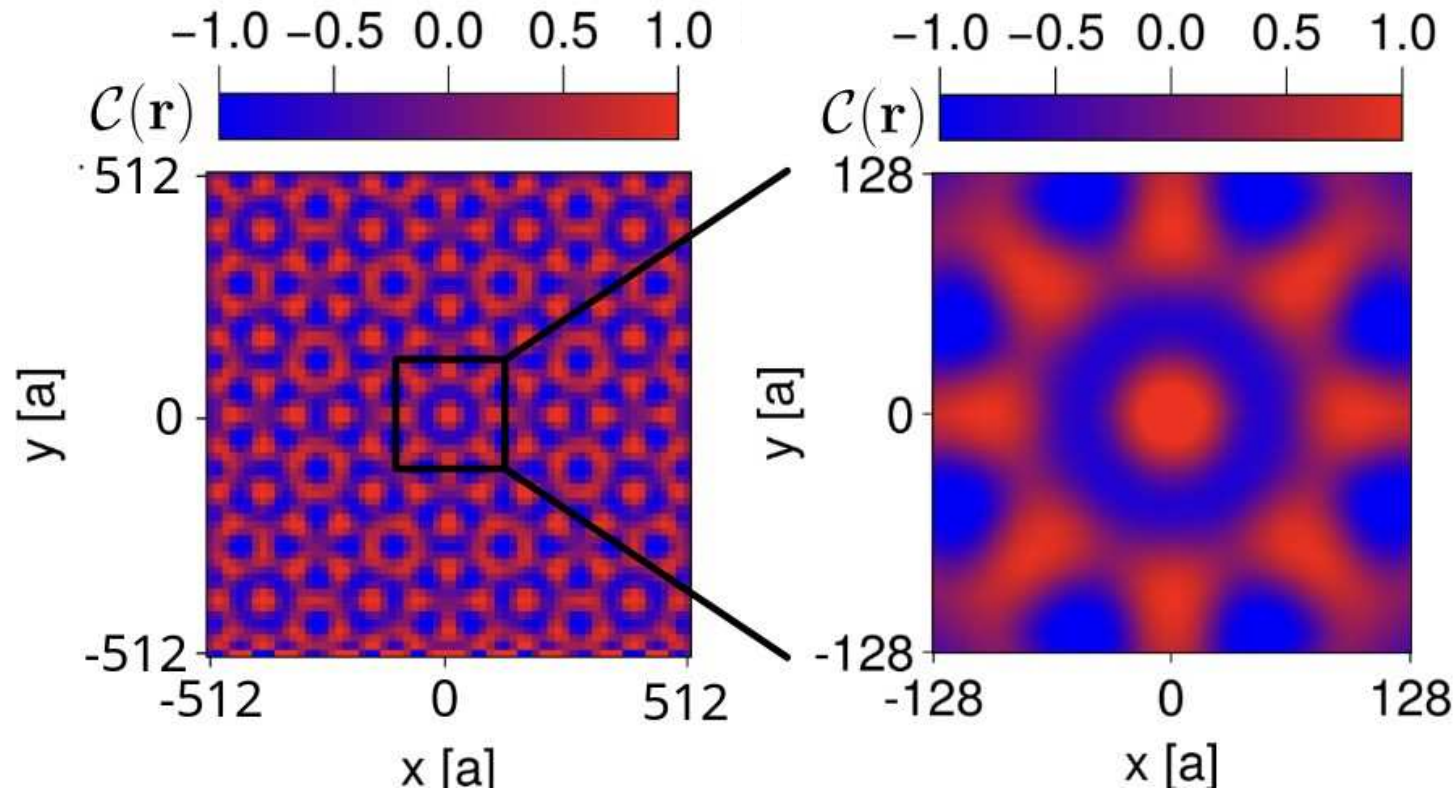
Real-space Chern number (Chern marker)

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

Tensor-network Chern marker

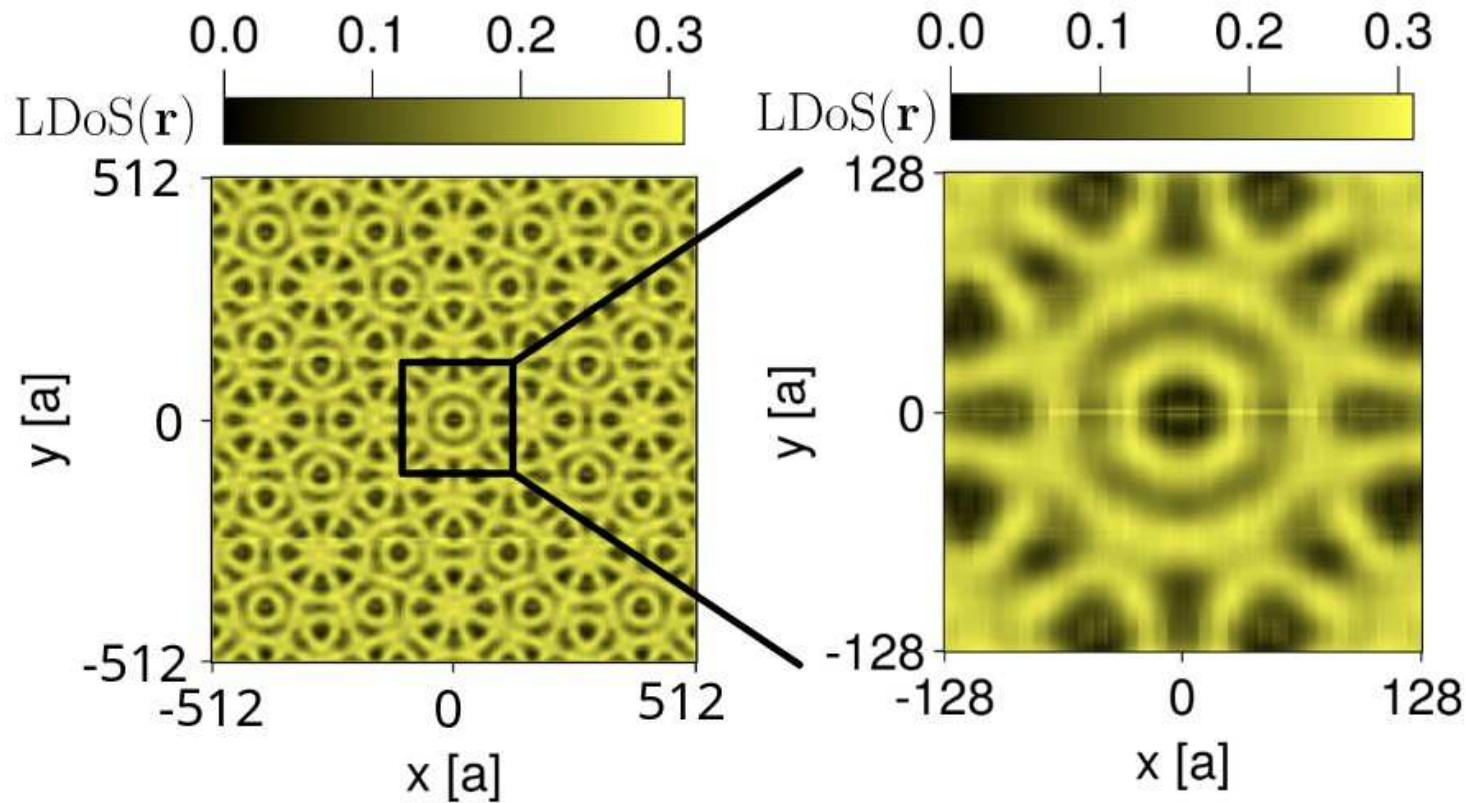
$$\hat{C}_{\alpha} = 2\pi i \left(\begin{array}{c} \hat{Q} \\ \hat{y}_{\alpha}^{\Lambda} \\ \hat{P} \\ \hat{x}_{\alpha}^{\Lambda} \\ \hat{Q} \end{array} \begin{array}{c} \text{---} \end{array} \begin{array}{c} \hat{P} \\ \hat{y}_{\alpha}^{\Lambda} \\ \hat{Q} \\ \hat{x}_{\alpha}^{\Lambda} \\ \hat{P} \end{array}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

Chern mosaic in a 8-fold topological quasicrystal



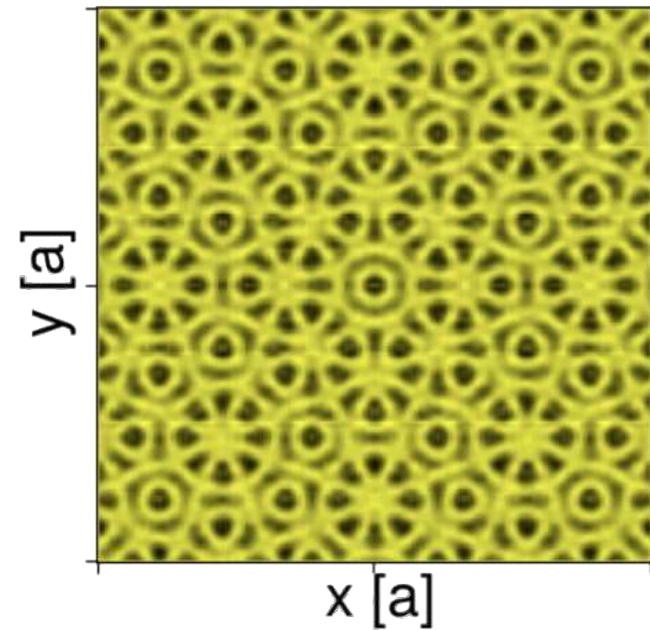
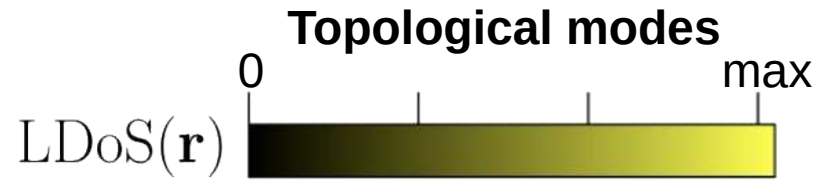
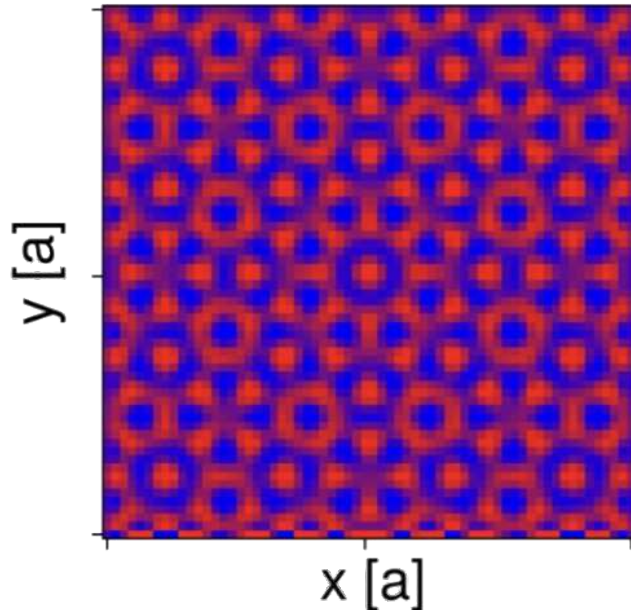
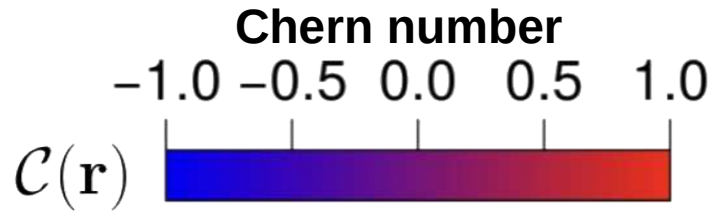
Domains with different topological invariants can be directly computed in real space

Topological modes in a 8-fold topological quasicrystal



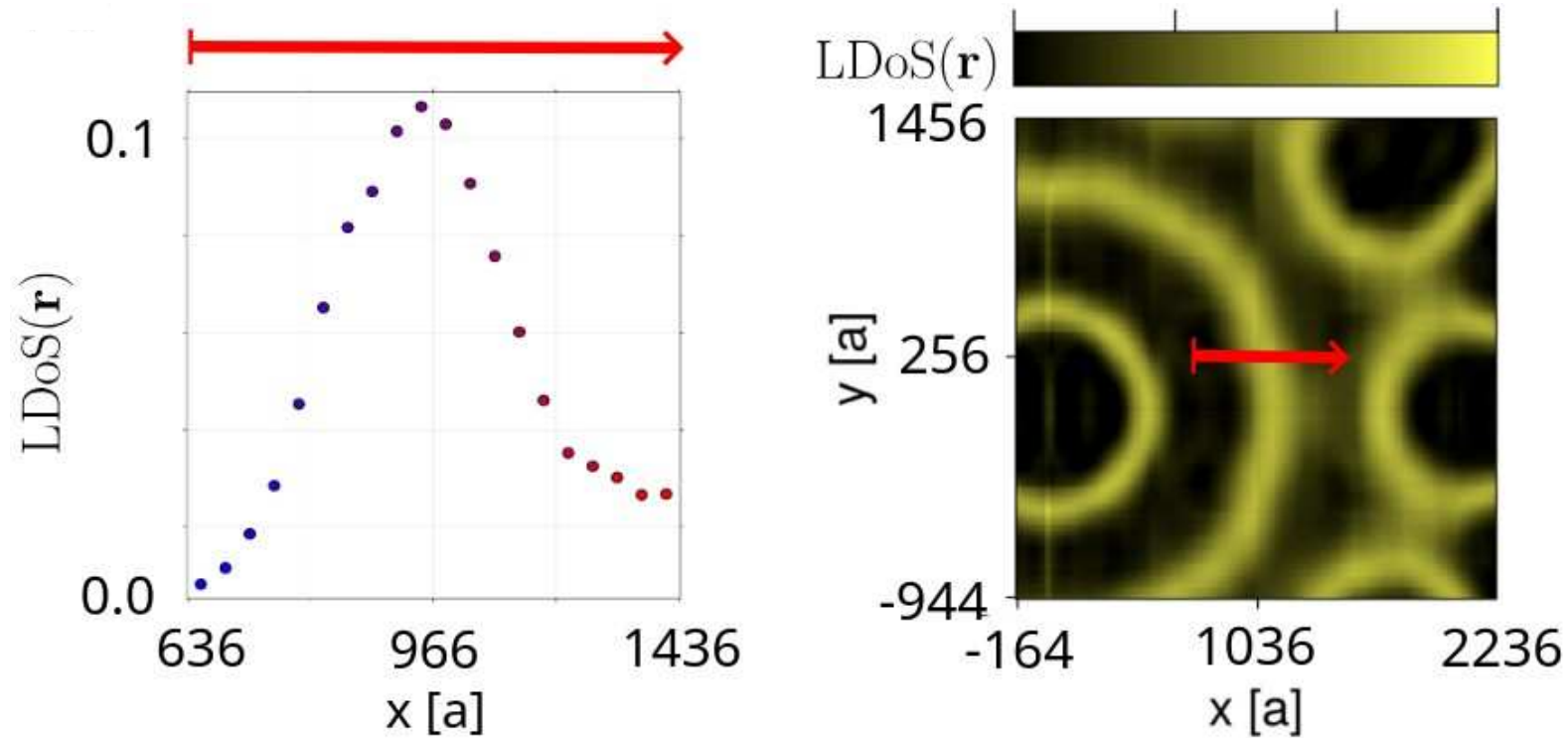
Topological modes appear between topological domains in real space

Chern mosaic and topological modes in a quasicrystal



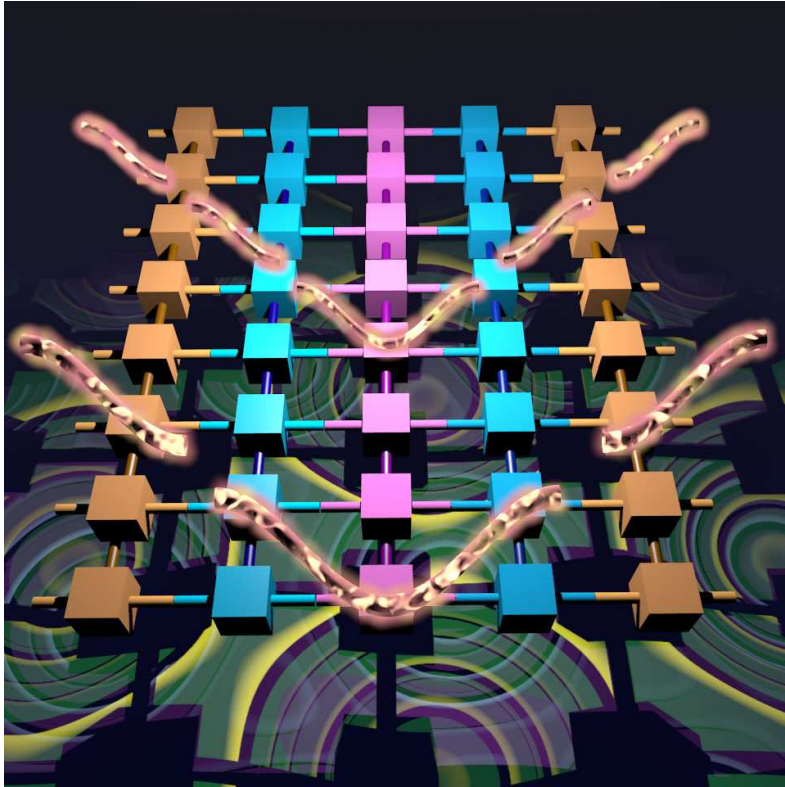
Tensor networks allow computing topology in exceptionally large super-moire systems

Zero modes across topological quasicrystalline domain



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

Tensor networks for momentum-resolved spectral functions



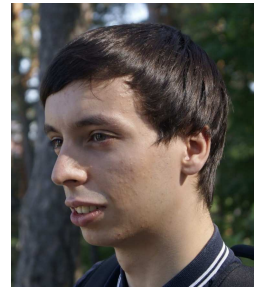
Anouar Moustaj



Yitao Sun



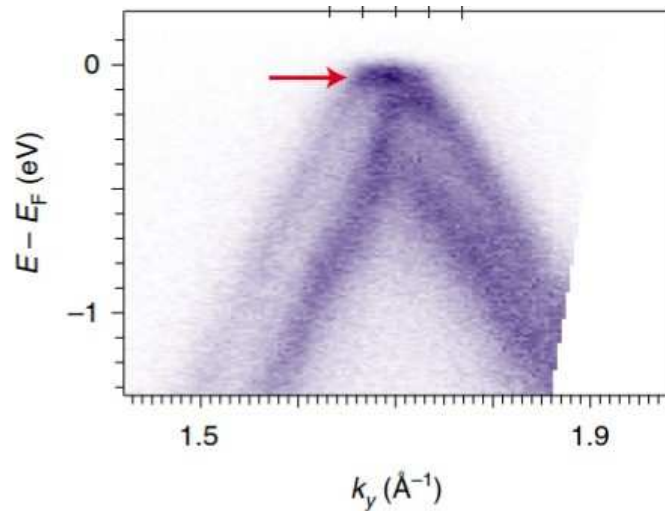
Tiago Antão



arXiv:2512.18397 (2025)

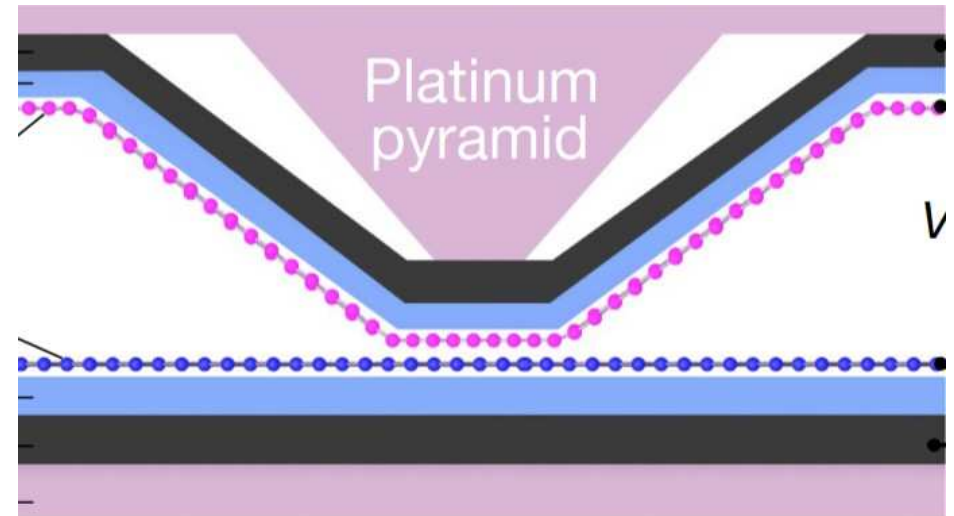
Momentum-resolved spectral functions

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

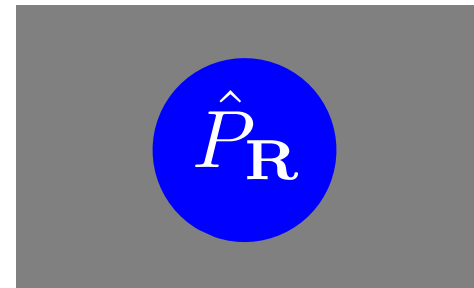
$$A_P(\mathbf{R}, \mathbf{k}, \omega) = \langle \mathbf{k} | \hat{\mathcal{F}} \hat{\mathcal{P}}_R \delta(\omega - \hat{\mathcal{H}}_{\text{MF}}) \hat{\mathcal{P}}_R \hat{\mathcal{F}}^{-1} | \mathbf{k} \rangle$$

Quantum Fourier transform

Projector in a (large-enough) region

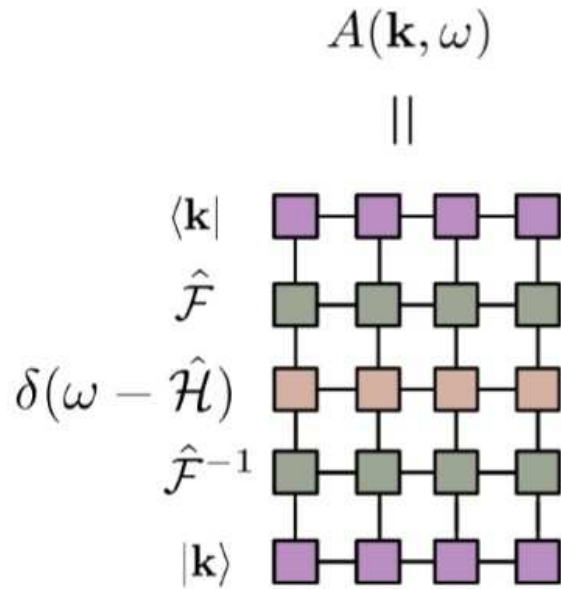
Tensor-network representation of the quantum Fourier transform

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

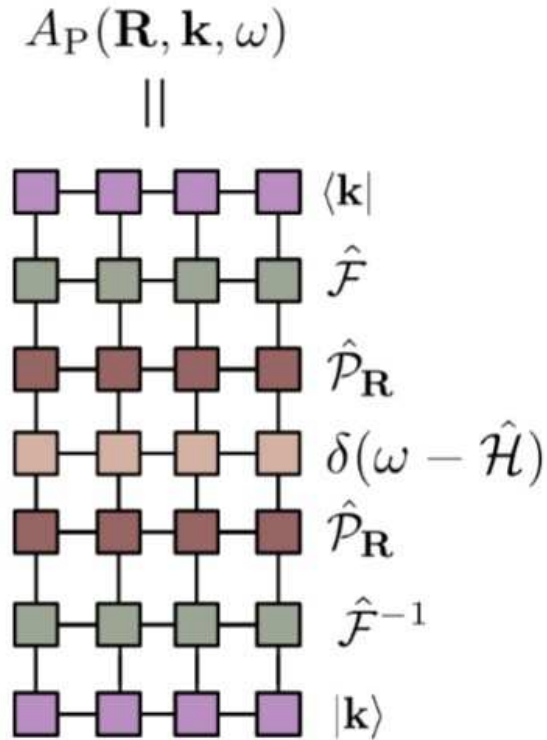


Tensor-network representation of the momentum-resolved spectral function

**Total momentum-resolved
spectral function**

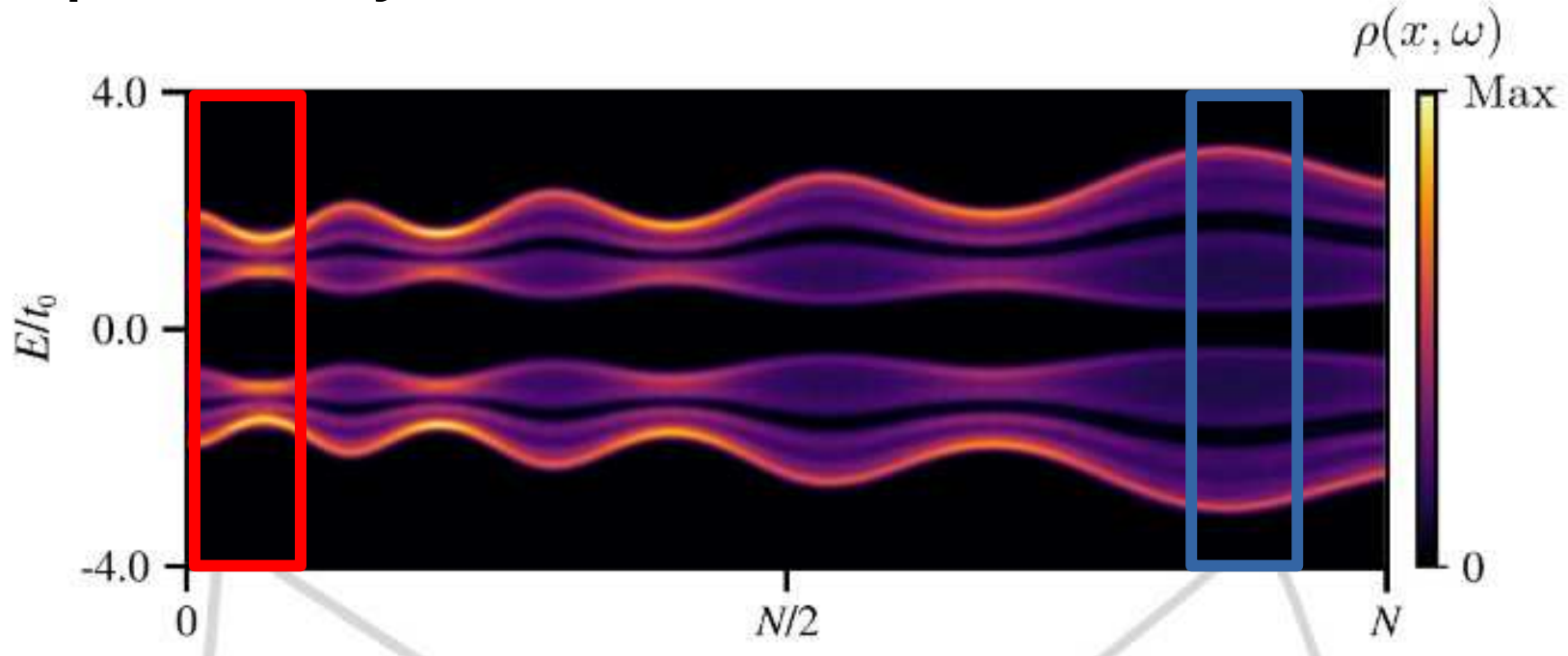


**Local momentum-resolved
spectral function**



Super-moire with non-uniform strain

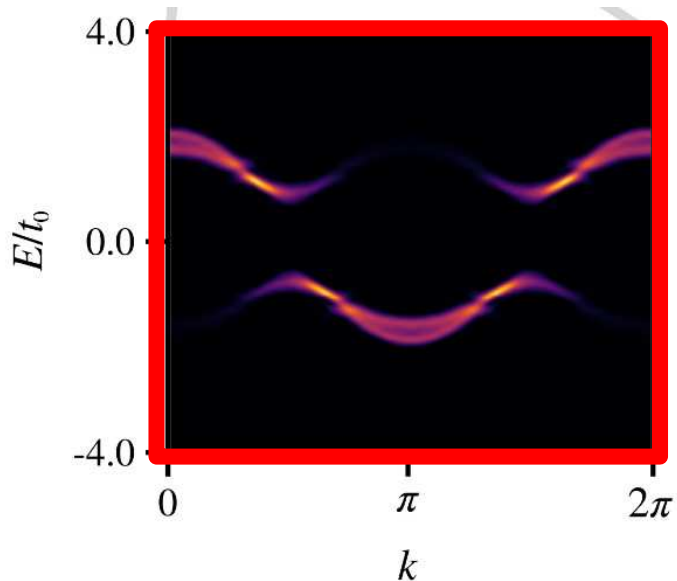
Super-moire system with non-uniform strain and interactions



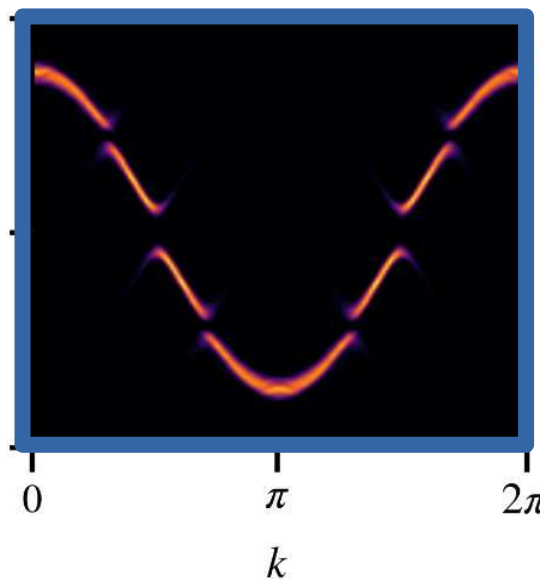
The super-moire features a strongly spatially-dependent electronic structure, that can be imaged in the local momentum-resolved spectral function

Super-moire with non-uniform strain

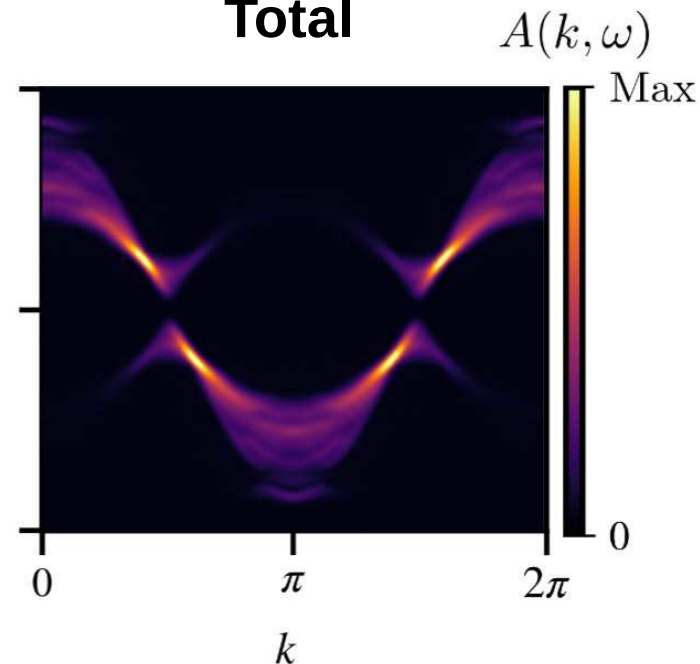
Region #1



Region #2



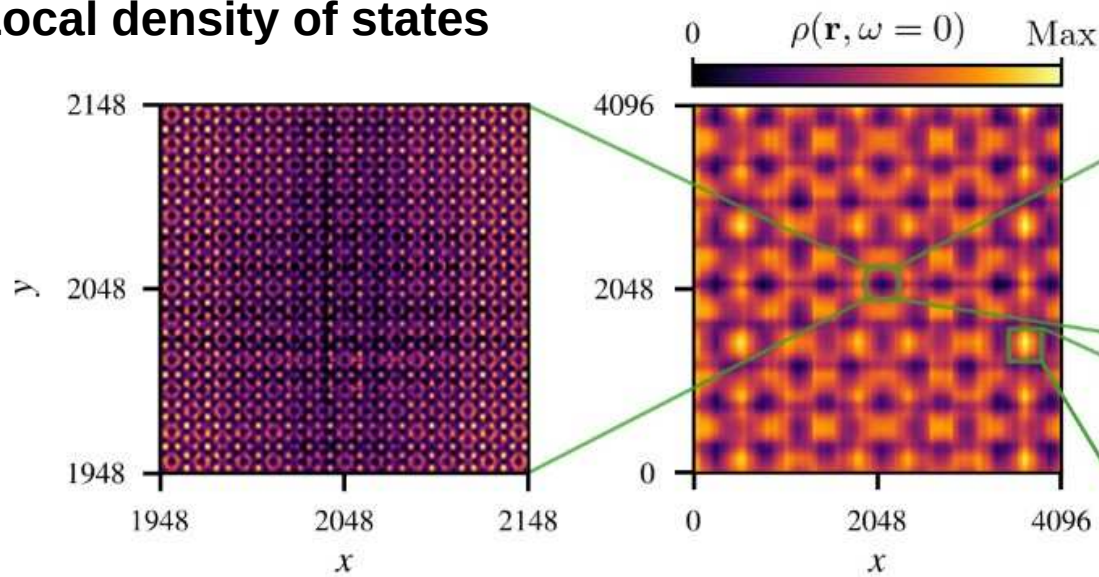
Total



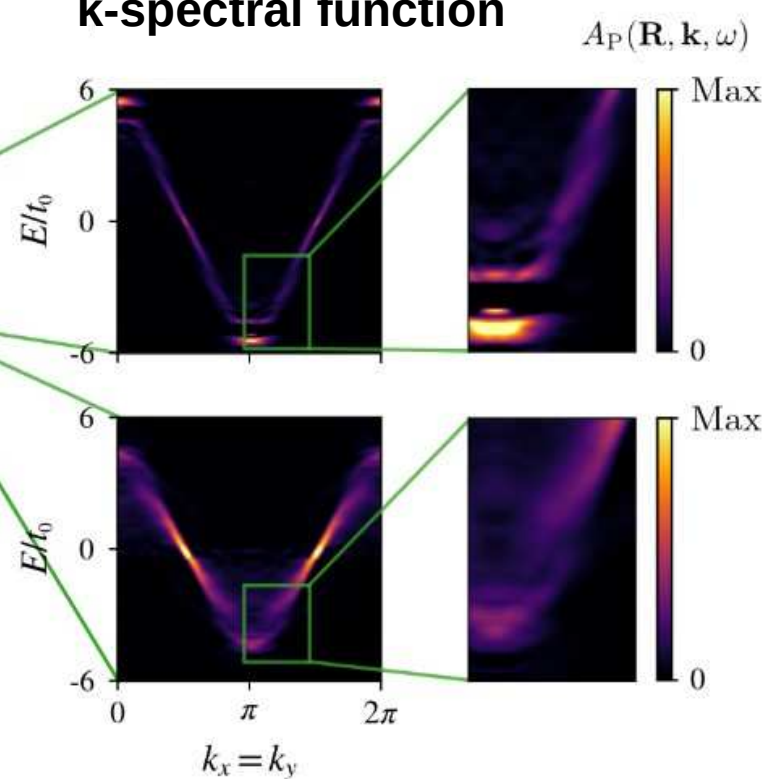
The super-moire features a strongly spatially-dependent electronic structure, that can be imaged in the local momentum-resolved spectral function

8-fold quasicrystal momentum-resolved functions

Local density of states

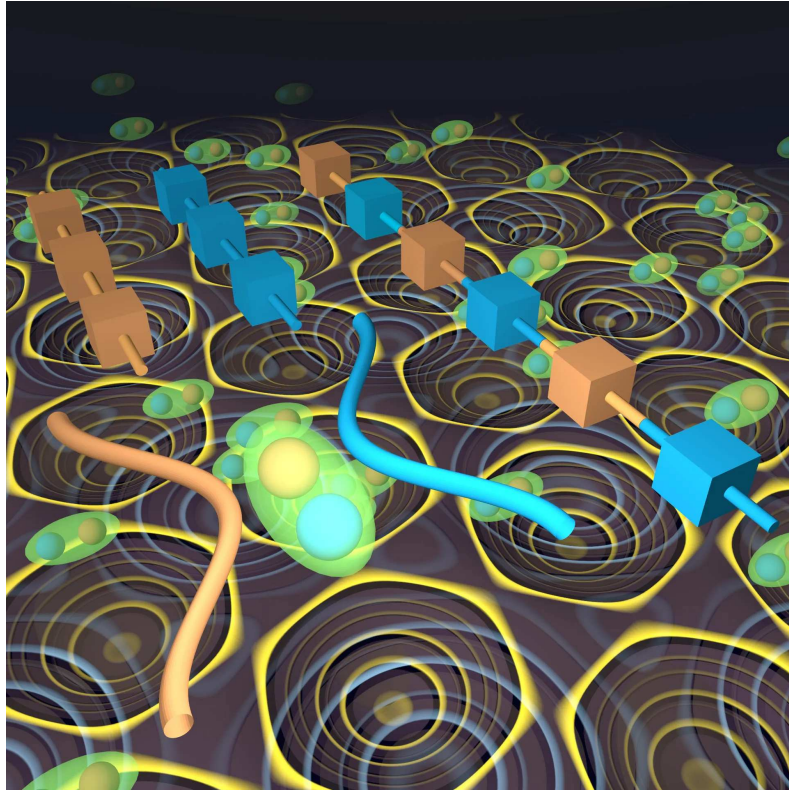


k-spectral function



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

Tensor-networks for super-moire excitons



arXiv:2603.02011 (2026)

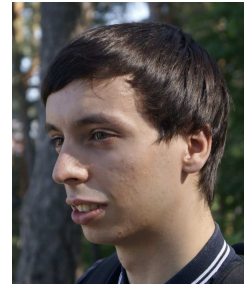
Anouar Moustaj



Yitao Sun



Tiago Antão

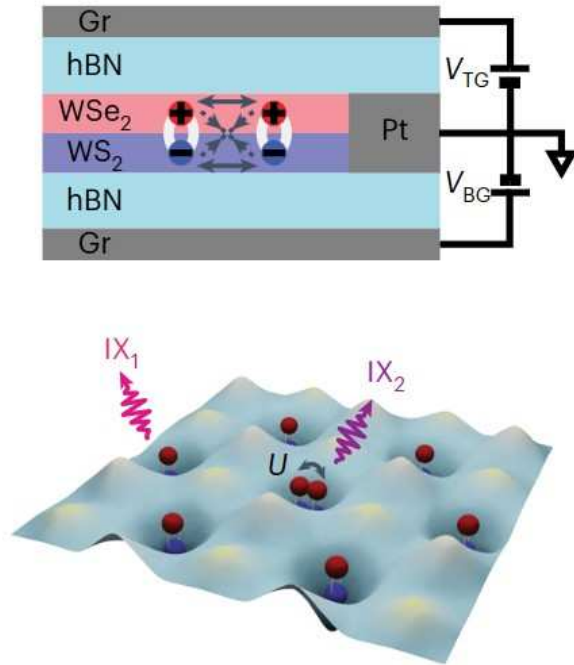


Lumen Eek

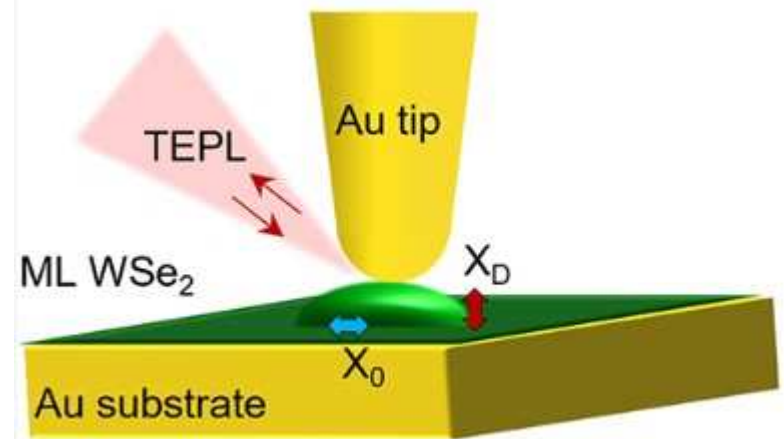


Excitons in super-moire systems

Strongly interacting excitons in moire superlattices



Local imaging of exciton in 2D materials

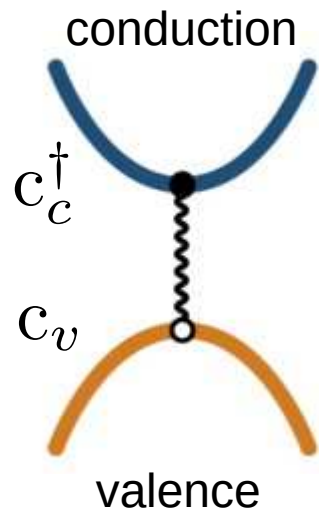


The challenge of computing excitons in moire systems

We take a typical (Hartree-Fock) electronic state $|\Omega\rangle = \prod_{\alpha \in \text{occ}} \psi_{\alpha}^{\dagger} |0\rangle$

Excitons are electron-hole bound pairs, that can be represented in the two-body basis

$$|n, m\rangle = c_{c,n}^{\dagger} c_{v,m} |\Omega\rangle \quad H_{\text{ex}} = \langle n, m | \mathcal{H} | n', m' \rangle$$



For a system with N sites, the two-particle state has a dimension of $\sim N^2$

For moire $N \sim 10^5 \rightarrow N^2 \sim 10^{10}$

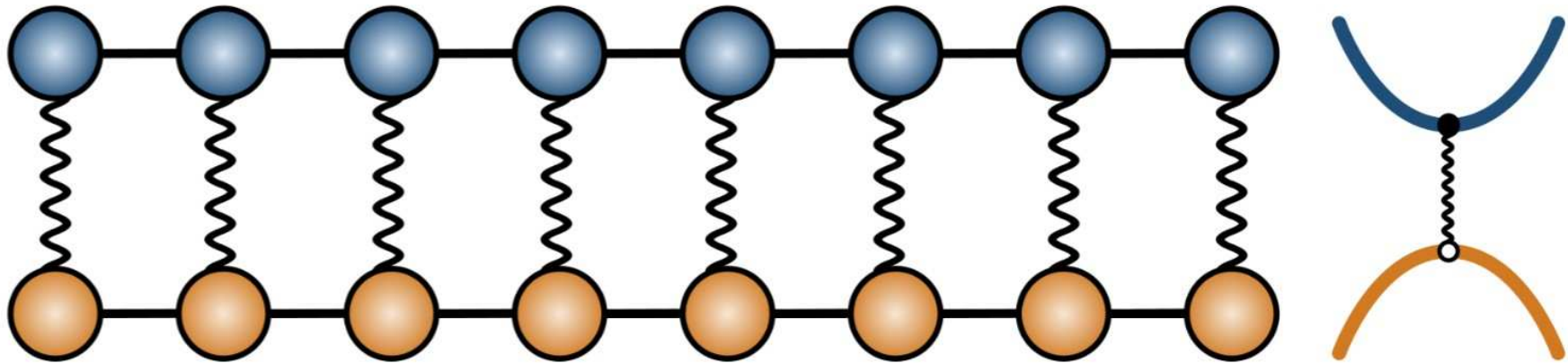
For super-moire $N \sim 10^9 \rightarrow N^2 \sim 10^{18}$

Even when single particle physics can be computed in moire two-particle physics becomes very quickly intractable

Mapping excitonic states to qubits

Let us start with a one dimensional semiconductor

$$c_{c,1}^\dagger|\Omega\rangle c_{c,2}^\dagger|\Omega\rangle c_{c,3}^\dagger|\Omega\rangle c_{c,4}^\dagger|\Omega\rangle c_{c,5}^\dagger|\Omega\rangle c_{c,6}^\dagger|\Omega\rangle c_{c,7}^\dagger|\Omega\rangle c_{c,8}^\dagger|\Omega\rangle$$



$$c_{v,1}|\Omega\rangle c_{v,2}|\Omega\rangle c_{v,3}|\Omega\rangle c_{v,4}|\Omega\rangle c_{v,5}|\Omega\rangle c_{v,6}|\Omega\rangle c_{v,7}|\Omega\rangle c_{v,8}|\Omega\rangle$$

How do we represent the exciton basis?

Mapping excitonic states to qubits

Electron-hole excitations over the ground state

$$c_{c,1}^\dagger c_{v,1} |\Omega\rangle, c_{c,1}^\dagger c_{v,2} |\Omega\rangle, \dots, c_{c,2}^\dagger c_{v,1} |\Omega\rangle, \dots, c_{c,8}^\dagger c_{v,8} |\Omega\rangle$$

$\updownarrow$ Pseudo-spin encoding

$$|\uparrow\uparrow\uparrow\uparrow\rangle, |\uparrow\uparrow\uparrow\downarrow\rangle, \dots, |\uparrow\downarrow\uparrow\uparrow\rangle, \dots, |\downarrow\downarrow\downarrow\downarrow\rangle$$

$$\begin{array}{ccc} H & & \hat{\mathcal{H}} \equiv \text{---} \square \text{---} \square \text{---} \square \text{---} \square \text{---} \square \text{---} \square \text{---} \\ 2^{2L} \times 2^{2L} & \xrightarrow{\text{Tensor network representation}} & 2L \text{ sites} \\ \text{Matrix} & & \text{Matrix Product Operator} \end{array}$$

We compute the local
exciton density of states

$$\rho(\mathbf{r}, E) = \langle \mathbf{r}, \mathbf{r} | \delta(E - \hat{\mathcal{H}}) | \mathbf{r}, \mathbf{r} \rangle$$

Mapping excitonic states to qubits

Original many-body Hamiltonian

$$\hat{H}_b = \sum_{l,m} t_{lm} c_{b,l}^\dagger c_{b,m} + \sum_l V_{b,l} c_{b,l}^\dagger c_{b,l}$$

$$\hat{H}_U = \sum_l U_l c_{c,l}^\dagger c_{c,l} c_{v,l}^\dagger c_{v,l},$$

Hamiltonian in the excitonic space

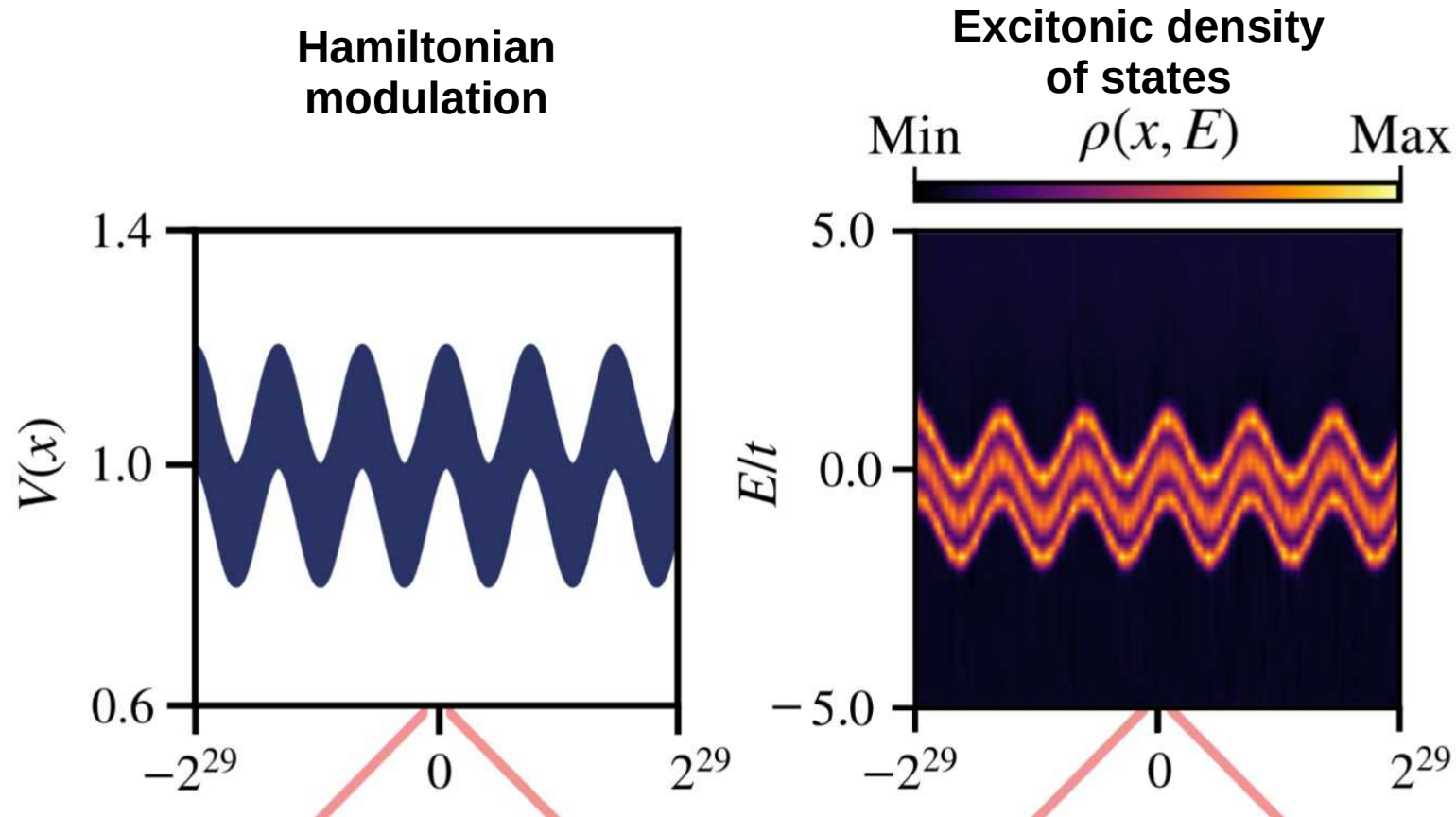
$$\hat{H}_X = \hat{T}_c \otimes \mathbb{1} - \mathbb{1} \otimes \hat{T}_v - \hat{U}$$

$$U_{klmn} = U_k \delta_{kl} \delta_{mn} \delta_{ln}$$

We compute the local
exciton density of states

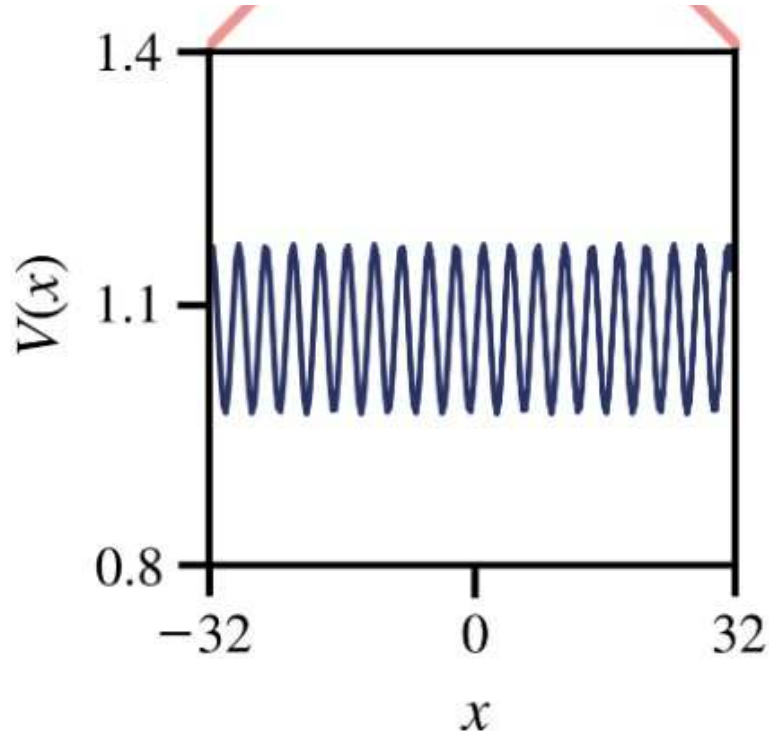
$$\rho(\mathbf{r}, E) = \langle \mathbf{r}, \mathbf{r} | \delta(E - \hat{\mathcal{H}}) | \mathbf{r}, \mathbf{r} \rangle$$

Local excitonic spectra of a 1D super-moire system

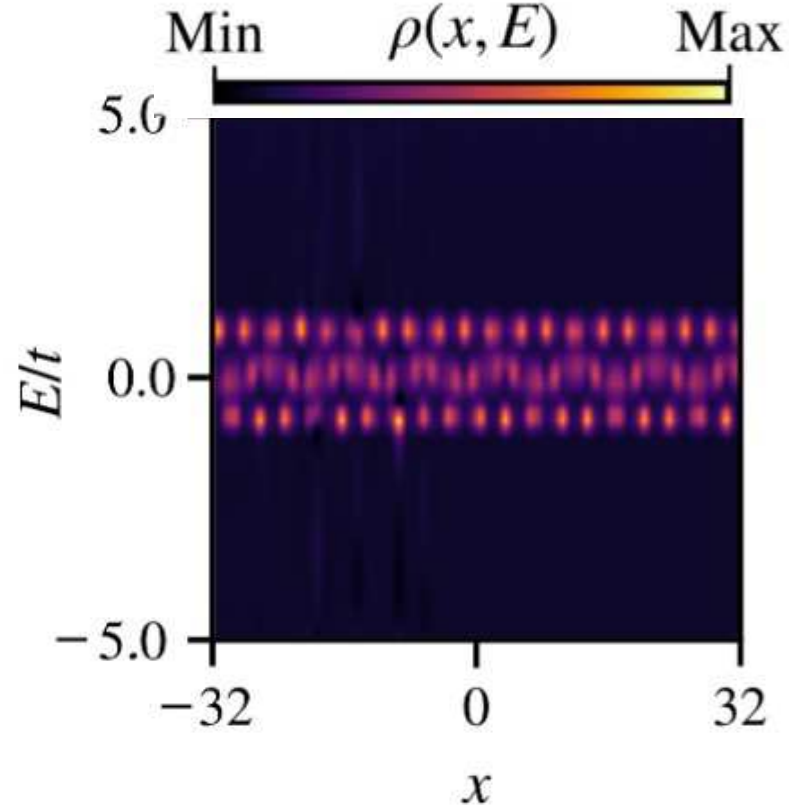


Local excitonic spectra of a 1D super-moire system

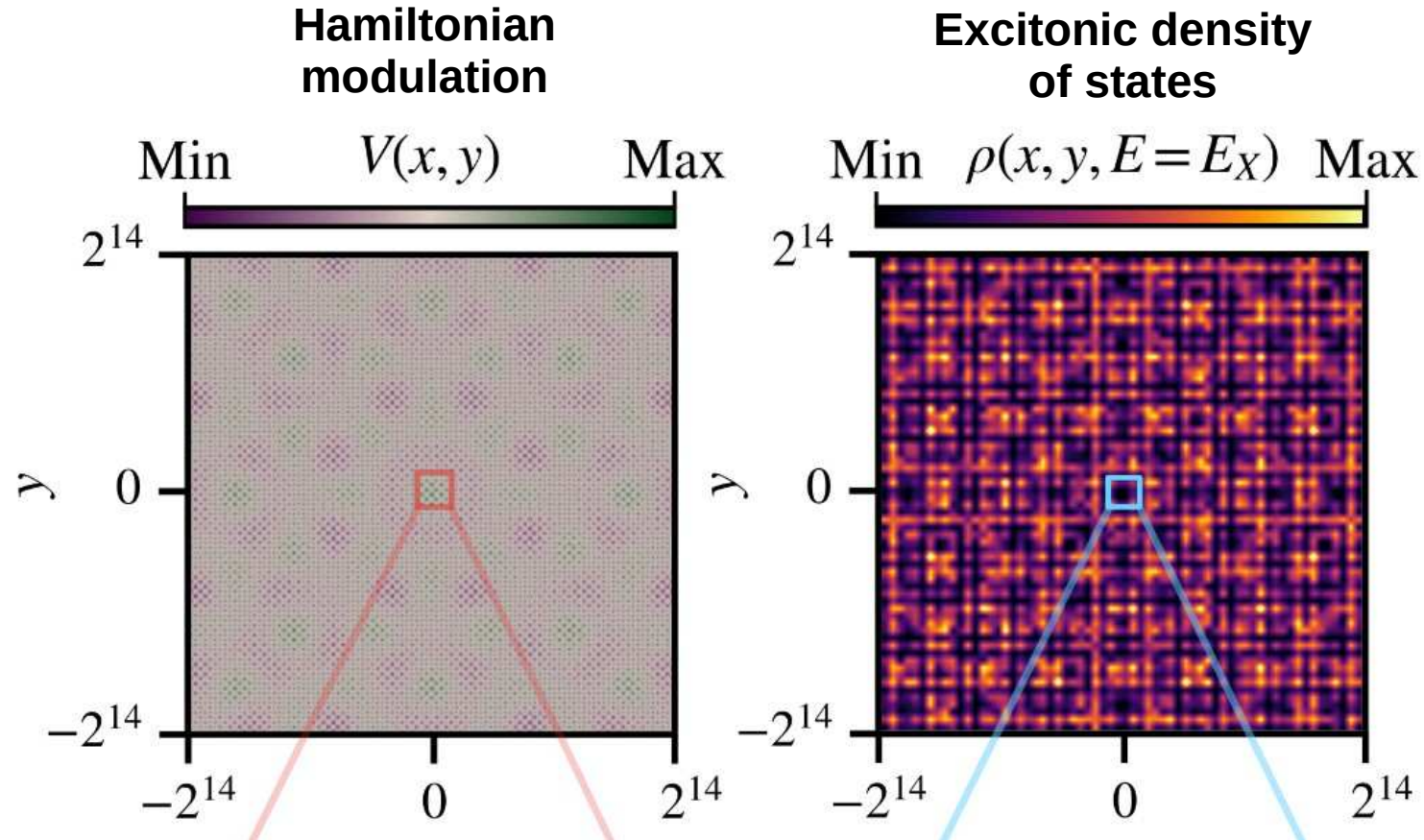
Hamiltonian modulation



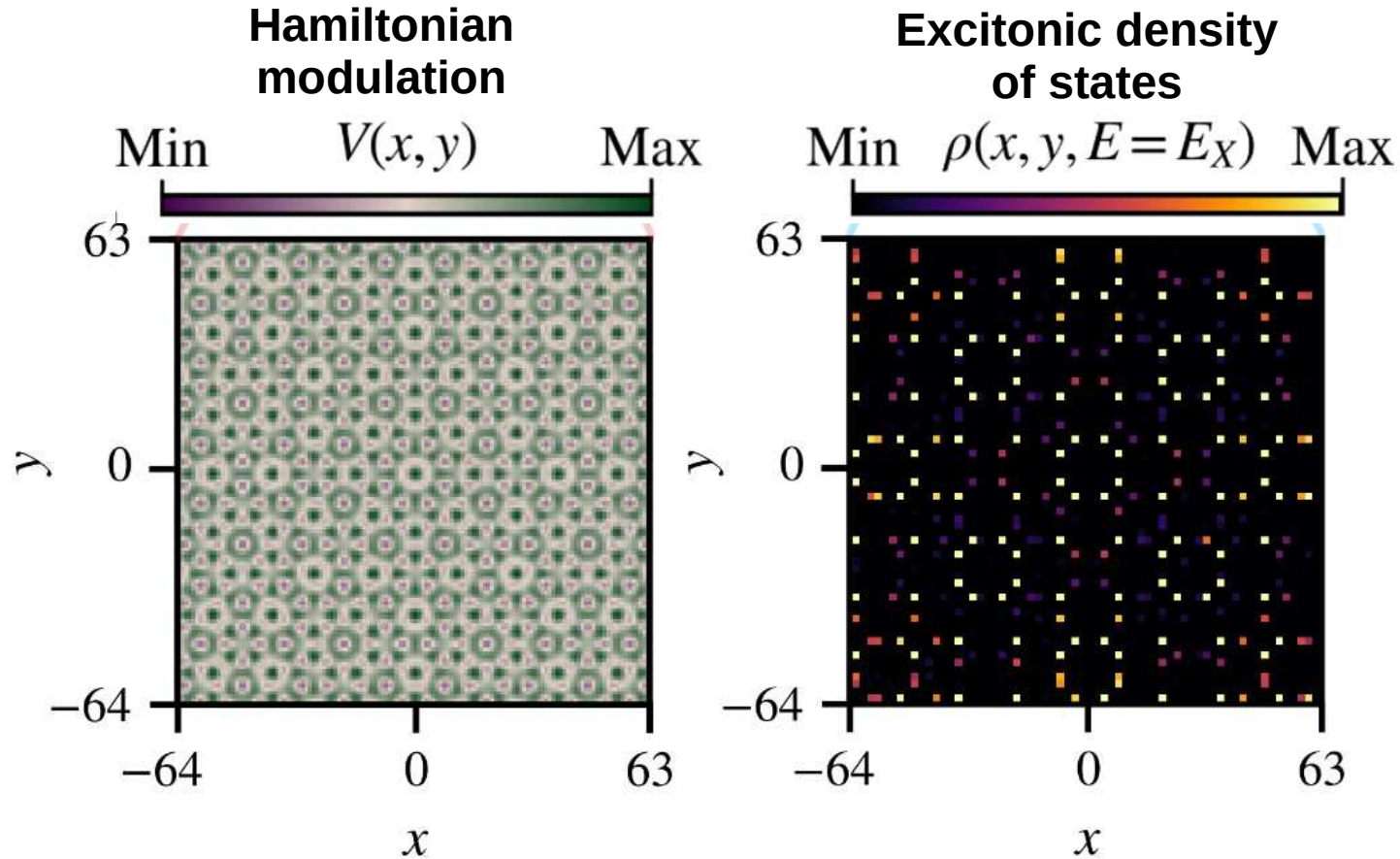
Excitonic density of states

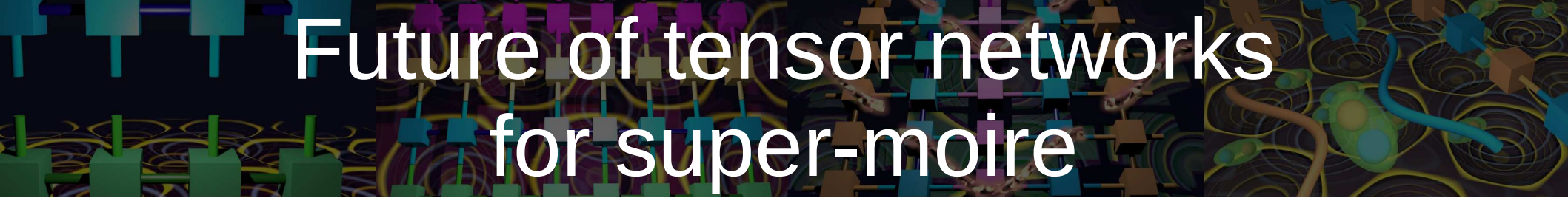


Local excitonic spectra of a 2D super-moire quasicrystal system



Local excitonic spectra of a 2D super-moire quasicrystal system





Future of tensor networks for super-moire

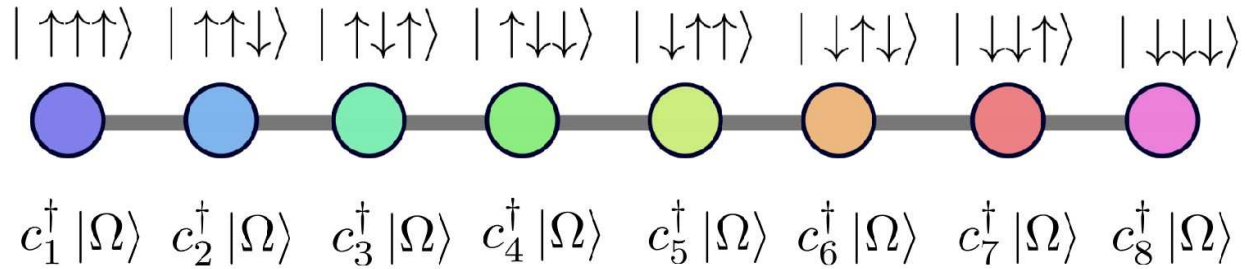
Potential future tensor network methods for super-moire

- 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)
- Dynamics of excitons, bi-excitons, trions

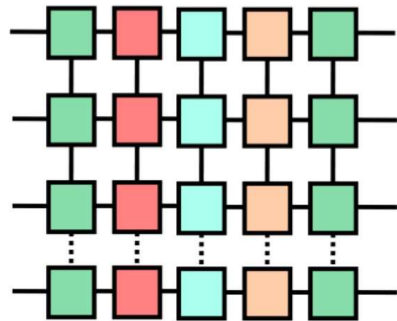
Effectively, anything that was possible with tight binding models for moderate systems, but now in moire and super-moire systems

Beyond tensor networks, super-moire matter in quantum computers

The mapping between tight binding sites and qubits could be directly implemented in a quantum circuit



Tensor network formulation

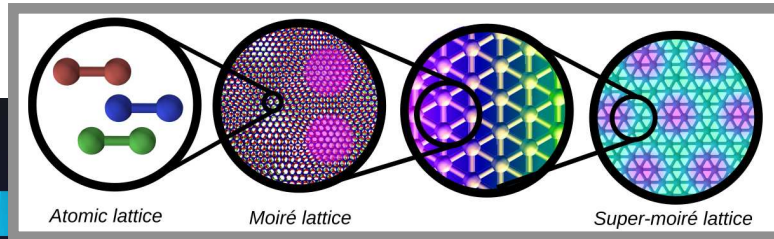


Quantum circuit formulation



Take home

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



Funding from

Finnish Quantum Flagship



Phys. Rev. Research 7, 043288 (2025)

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

arXiv:2512.18397 (2025)

arXiv:2603.02011 (2026)

