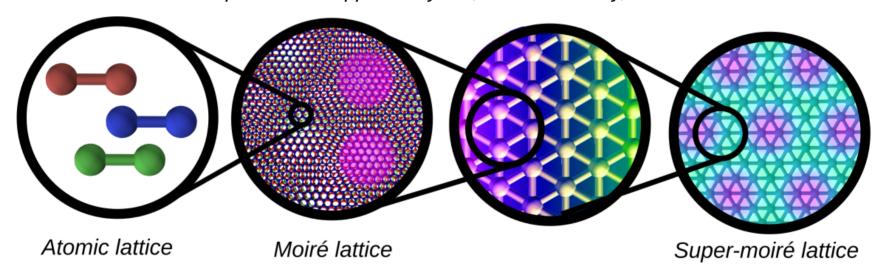
Solving topological and correlated super-moire materials with tensor networks and tensor cross interpolation

Jose Lado

Department of Applied Physics, Aalto University, Finland



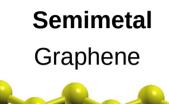
2D Materials 12 (1), 015018 (2025)

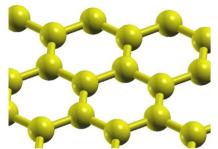
arXiv:2503.04373 (2025)

arXiv:2506.05230 (2025)

International workshop on tensor cross interpolation and other algorithms to learn tensor networks Grenoble, France, October 6th 2025

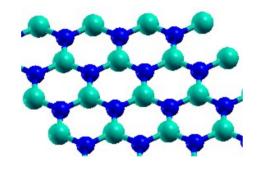
The two-dimensional materials world



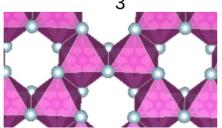


Semiconductor WS₂

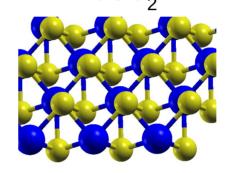
Insulator BN



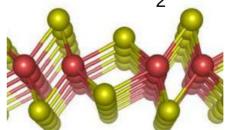
Ferromagnet Crl₃



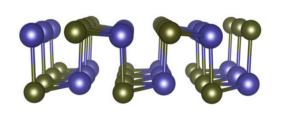
Superconductor NbSe₂



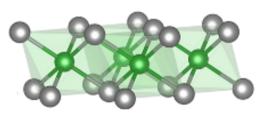
Quantum spin Hall insulator WTe₂



Ferroelectric SnTe

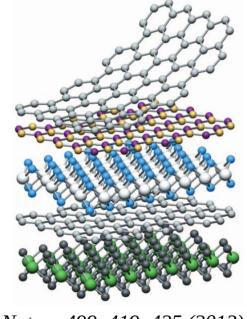


Multiferroic Nil₂



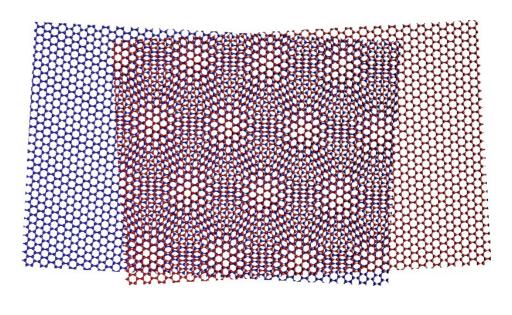
The flexibility of two-dimensional materials

They can be stacked



Nature 499, 419-425 (2013)

They can be rotated

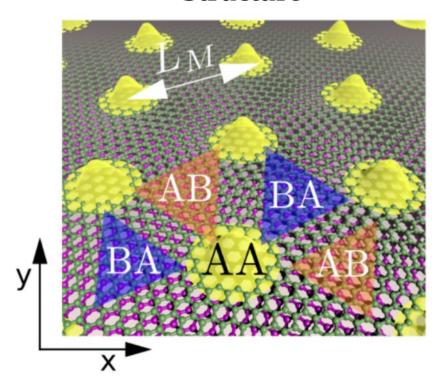


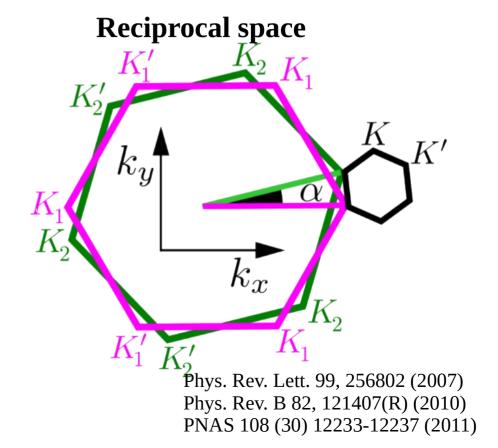
Science 361, 6403, 690-693 (2018)

These are unique features of two-dimensional materials

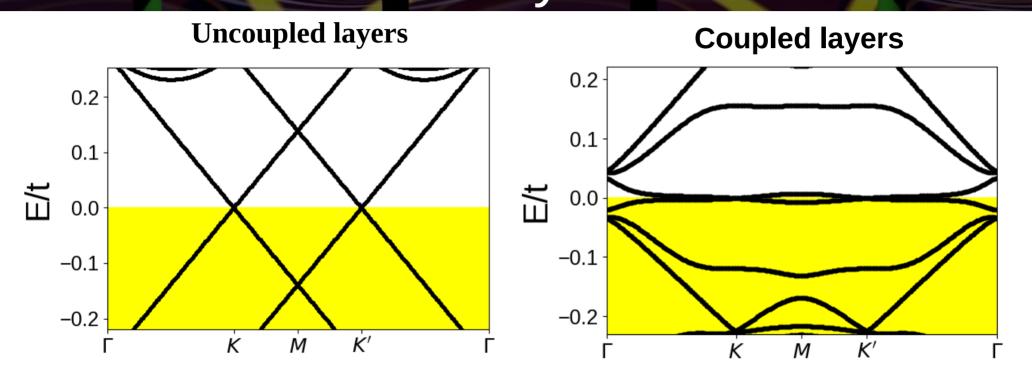
Twisted graphene bilayers

Structure





Electronic structure of twisted bilayer

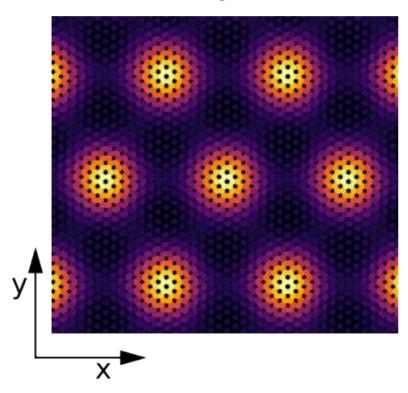


Twisted graphene bilayers feature flat bands driven by the twist

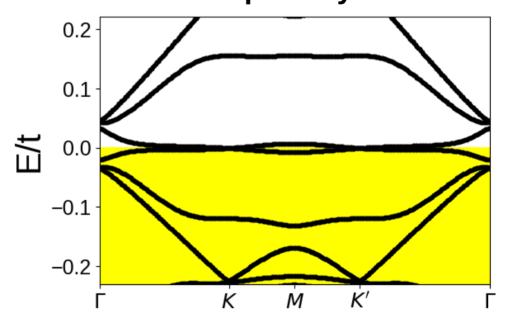
Phys. Rev. Lett. 99, 256802 (2007) Phys. Rev. B 82, 121407(R) (2010) PNAS 108 (30) 12233-12237 (2011)

Electronic structure of twisted bilayer

Local density of states



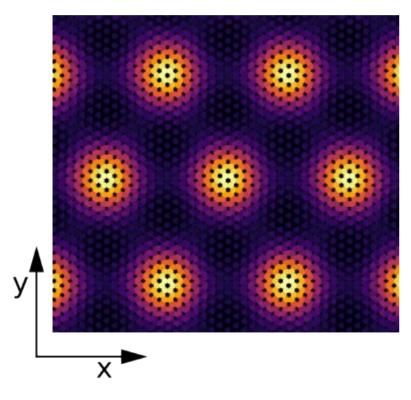
Coupled layers



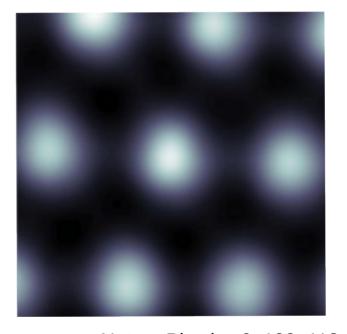
Phys. Rev. Lett. 99, 256802 (2007) Phys. Rev. B 82, 121407(R) (2010) PNAS 108 (30) 12233-12237 (2011)

Electronic structure of twisted bilayer

Local density of states

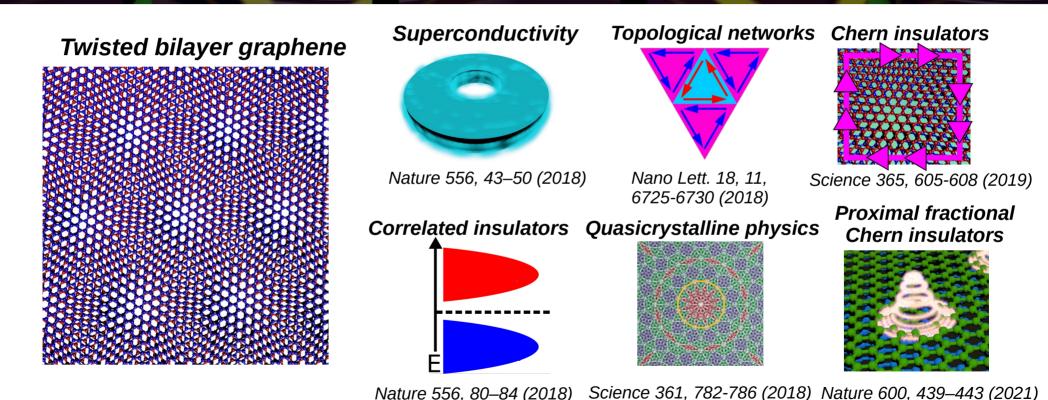


Experimental local density of states



Nature Physics 6, 109–113 (2010) Nature 572, 101–105 (2019) Nature 572, 95–100 (2019)

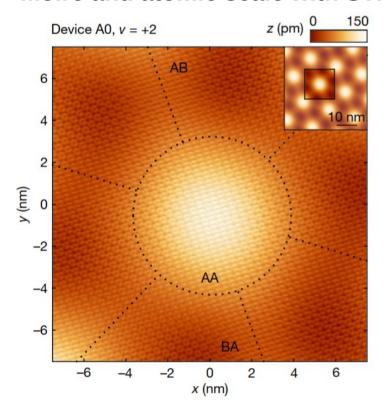
The tunability of twisted van der Waals materials



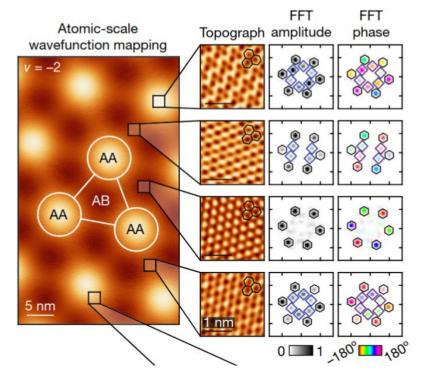
Twisted multilayers provide a powerful platform for emergent phenomena

Experimental observation of multiple scales in twisted bilayers

Moire and atomic scale with STM



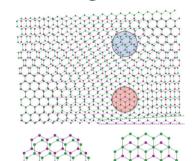
Atomic-scale symmetry breaking with STM



Nature 620, 525-532 (2023)

Artificial quantum matter in moire van der Waals heterostructures

Unconventional magnets

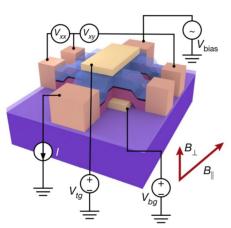


Twisted CrBr₃

YORK YORK

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

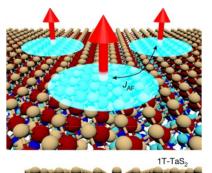
Unconventional superconductors

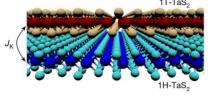


Twisted trilayer graphene

Nature 595, 526–531 (2021)

Heavy-fermion quantum materials

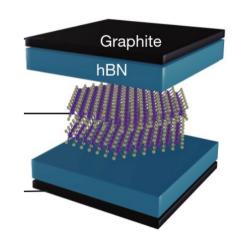




1H-1T TaS₂

Nature 599, 582–586 (2021)

Fractional topological matter

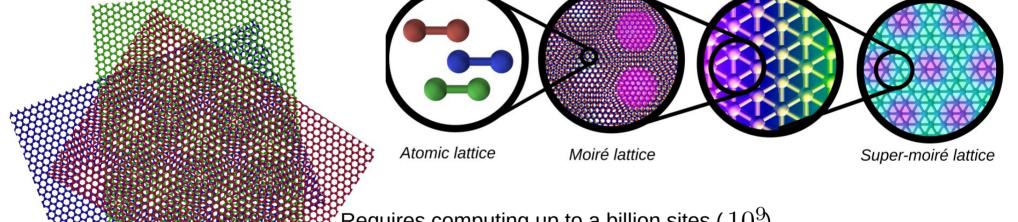


Twisted MoTe₂

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)

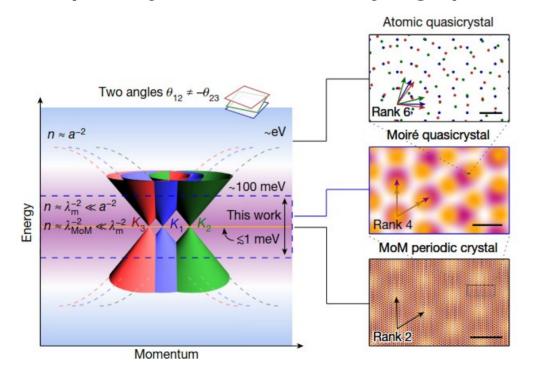
Experiments showing correlations and unconventional superconductivity

Nature 620, 762–767 (2023) Nature 625, 494–499 (2024) Nature 641, 896–903 (2025)

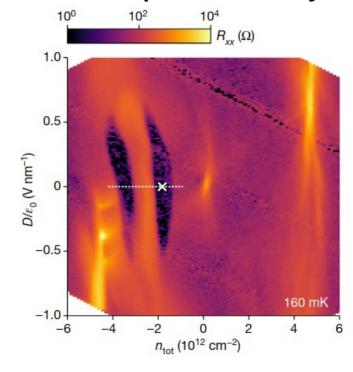
How can we compute the electronic structure of exceptionally large systems?

Super-moire materials, experimentally

Moire quasicrystal in twisted trilayer graphene

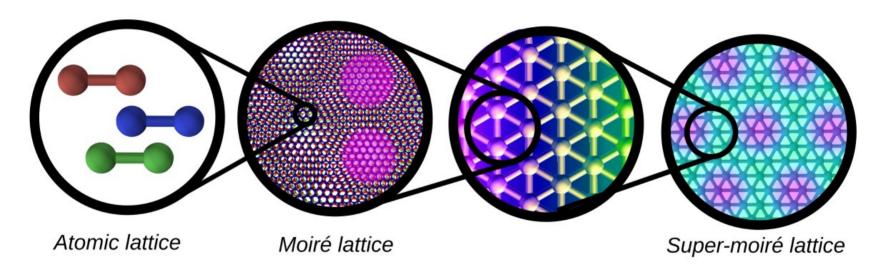


Coexisting correlations and superconductivity



Nature 620, 762-767 (2023)

Why super-moire materials are hard (for theorists)



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

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

(even going beyond usual memory limitations of conventional methods)

Behind the scenes

Yitao Sun



Tiago Antão



Marcel Niedermeier



Adolfo Fumega



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

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

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

Tensor networks for interacting super-moire materials

Modeling electrons in a material

Define operators that can create or destroy particles

$$\mathcal{C}_i$$
 Annihilation operator, destroys a particle in site i

$$C_i^{\dagger}$$
 Creation operator, creates a particle in site i

The empty vacuum state
$$|\Omega\rangle$$
 is defined as $|c_i|\Omega\rangle=0$

The Hamiltonian is written in terms of creation and annihilation operators

$$H = c_0^{\dagger} c_1 + h.c.$$

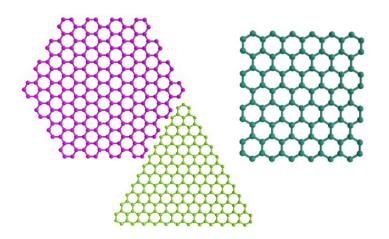
Modes in a single particle Hamiltonian

To solve a single particle Hamiltonian, we just have to diagonalize the matrix

$$H = \sum_{ij} t_{ij} c_i^{\dagger} c_j$$

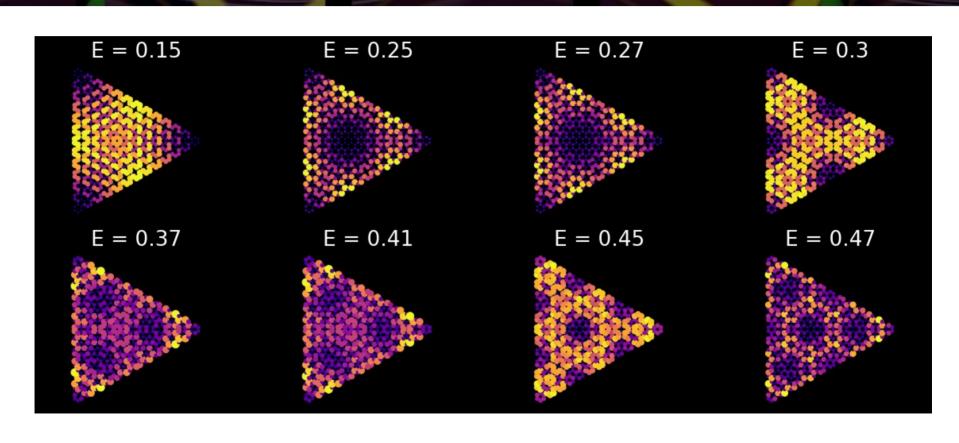
$$H = \sum_{\alpha} \epsilon_{\alpha} \Psi_{\alpha}^{\dagger} \Psi_{\alpha}$$

If take a certain finite geometry, we can find the confined modes

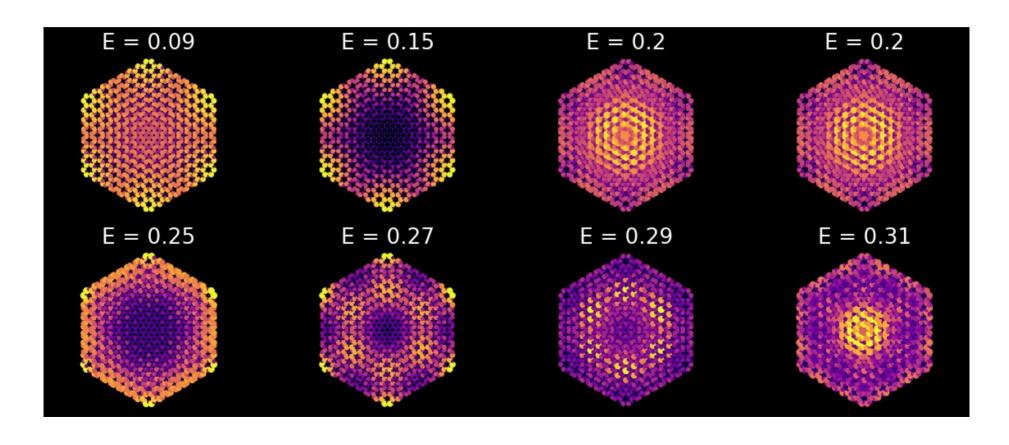


Let us do it for graphene islands

Confined modes in graphene islands



Confined modes in graphene islands



The challenge of correlated super-moire materials

Hamiltonian describing electrons in a super-moire material

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

Mean-field treatment of the interacting Hamiltonian

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

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

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

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

Tensor network for single particle tight binding problems

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

We can use tensor networks to solve very large tight binding problem

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

arXiv:2503.04373 (2025)

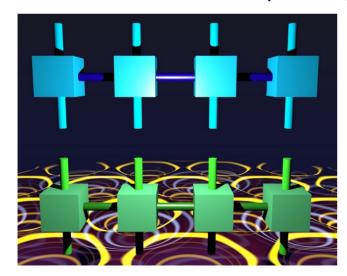
arXiv:2506.05230 (2025)

Dealing with very large spaces with tensor networks

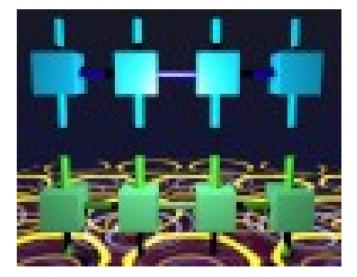
A many-body wavefunction a is a very high dimensional object (2^L coefficients)

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

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

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

We need to determine in total $\,2^L\,$ coefficients

Is there an efficient way of storing so many coefficients?

Tensor networks allow parametrizing many-body wavefunctions as

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

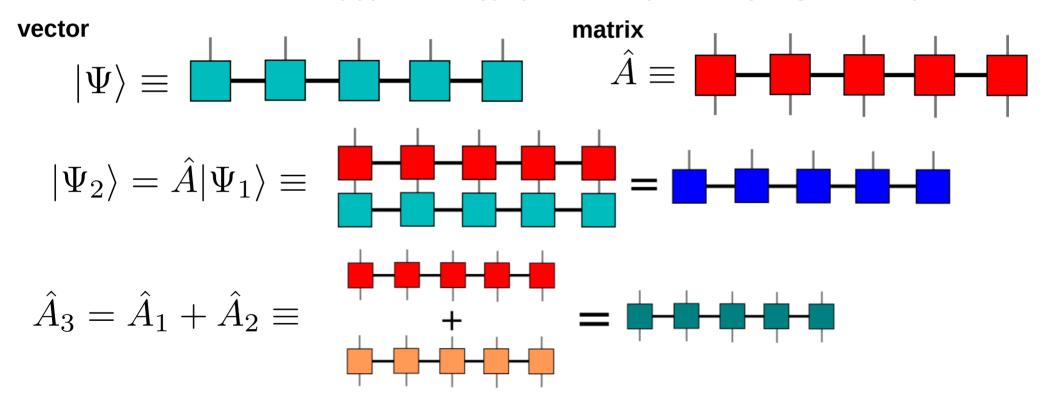
$$L\chi^2 \ \ {\rm parameters}$$
 Full wavefunction
$$\thickapprox \ Matrix\ {\it product\ state}$$

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



Learning the tensor network representation

We need to represent all the tight binding terms as tensor networks

- In some cases, we can build the initial tensor network explicitly
- In other cases, we learn the tensor network with quantics tensor cross interpolation

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

SciPost Phys. 18, 104 (2025)

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

$$H^{MF} = \sum_{\alpha\beta} (t_{\alpha\beta} + \chi_{\alpha\beta}) c_{\alpha}^{\dagger} c_{\beta} = \sum_{\alpha\beta} H_{\alpha\beta}^{MF} c_{\alpha}^{\dagger} c_{\beta} \qquad \mathcal{H}_{\alpha\beta}^{MF} \equiv \begin{array}{c} \downarrow \\ \downarrow \\ \downarrow \end{array} - \begin{array}{c} \downarrow \\ \downarrow \end{array}$$

Tensor network representation of the correlators

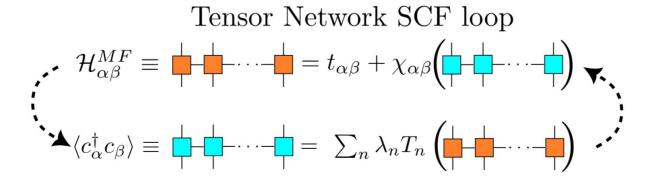
$$\langle c_{\alpha}^{\dagger} c_{\beta} \rangle = \langle \alpha | \Xi(\mathcal{H}^{MF}) | \beta \rangle \equiv$$

Self-consistent electronic interactions with tensor networks

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

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

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



Spectral functions with the kernel polynomial method

Let us expand a delta function in Chebyshev polymials

$$\delta(\omega - \mathcal{H}) = \sum_{n} \lambda_n(\omega) T_n(\mathcal{H})$$

Chebyshev relation

$$T_n(\mathcal{H}) = 2\mathcal{H}T_{n-1}(\mathcal{H}) - T_{n-2}(\mathcal{H})$$

Expansion coefficients for delta function

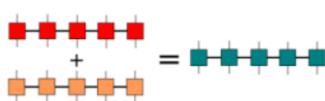
$$\lambda_n(\omega) = \frac{2T_n(\omega)}{\pi\sqrt{1-\omega^2}}$$

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

KPM can be implemented with tensor networks by using tensor network algebra

Phys. Rev. B 83, 195115 (2011)

Phys. Rev. Research 1, 033009 (2019)



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)

Tensor network representation of a super-moire 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

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

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 fo the modulation and store in a diagonal MPO $\,\mathcal{T}\,$

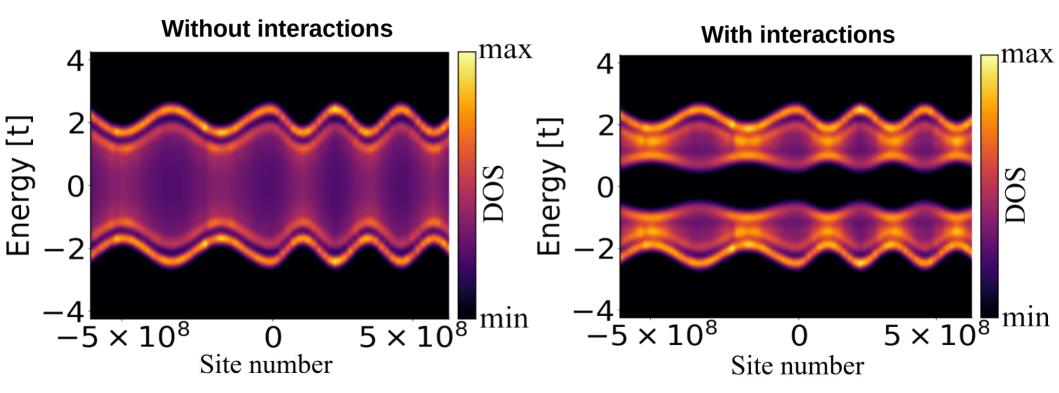
$$|\tau\rangle = \sum M_{s_1}^{(1)} M_{s_2}^{(2)} M_{s_3}^{(3)} ... M_{s_L}^{(L)} |s_1, s_2, ..., s_L\rangle$$

Quantics tensor cross interpolation

Modulated super-moire by constraction

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

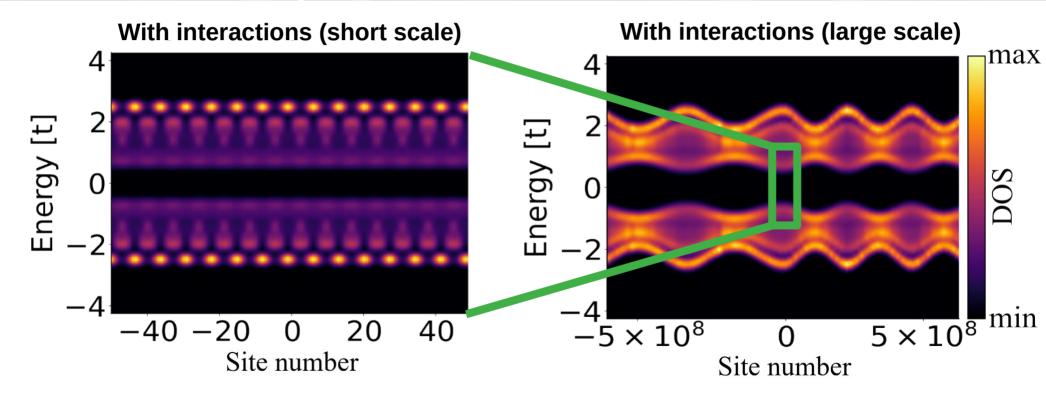
Solving billion-size super-moire materials



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

arXiv:2503.04373 (2025)

Solving billion-size super-moire materials

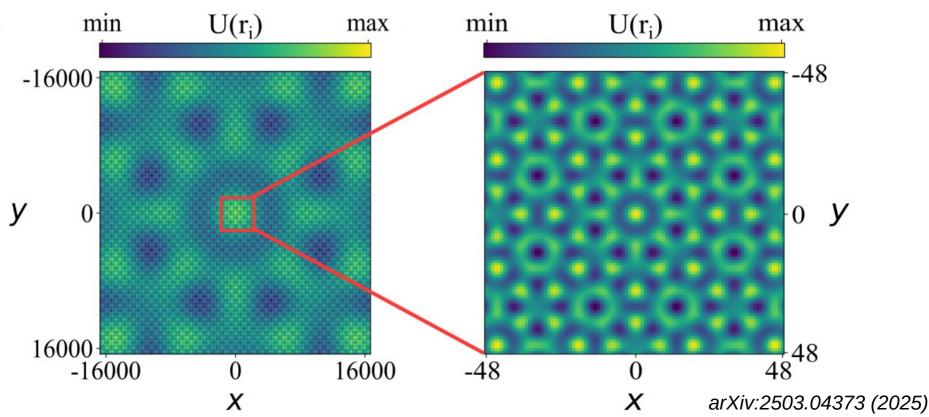


Tensor networks allow to solve selfconsistently a super-moire with one billion sites

arXiv:2503.04373 (2025)

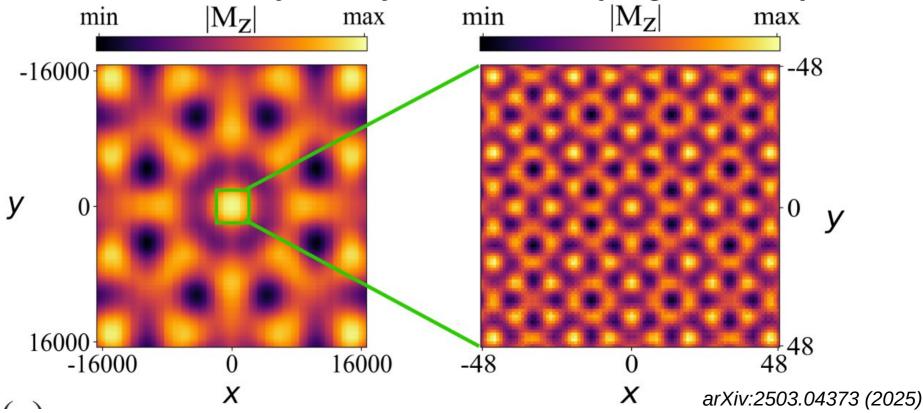
Two-dimensional billion size interacting super-moire

Modulation fo the Hamiltonian

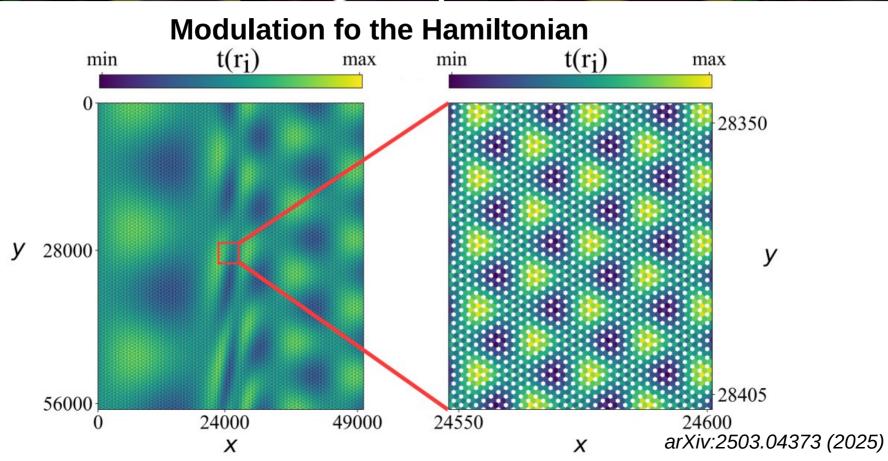


Two-dimensional billion size interacting super-moire

Selfconsistent symmetry broken order (magnetization)

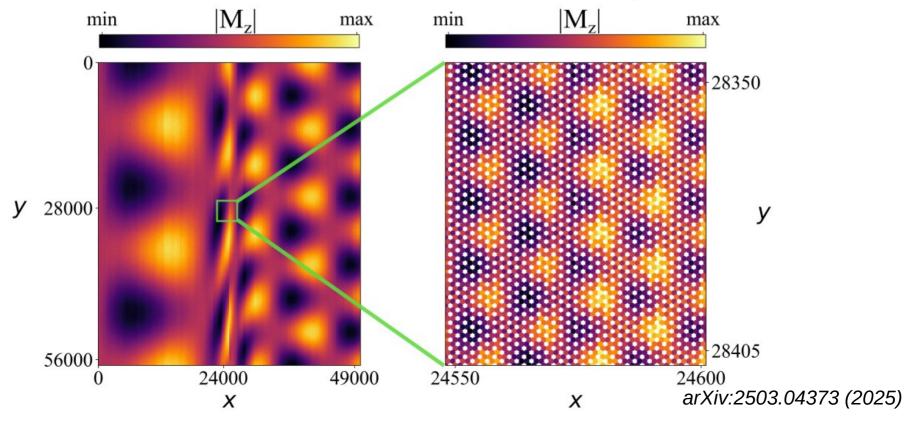


Two-dimensional billion size interacting super-moire



Two-dimensional billion size interacting super-moire

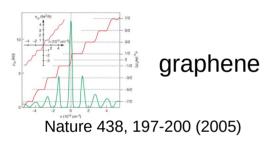
Selfconsistent symmetry broken order (magnetization)



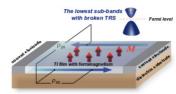
Tensor networks for topological super-moire materials

Topological quantum matter

Quantum Hall effect



Quantum Anomalous Hall effect

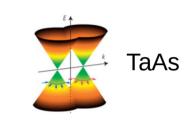


Cr-doped $(Bi,Sb)_2Te_3$

Fe@Pb

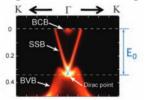
Science 340.6129 (2013): 167-170

Weyl semimetal



Nature Physics 11, 724–727 (2015)

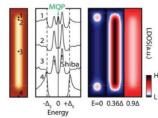
Quantum Spin Hall effect



Bi₂Se₃

Science 325.5937 (2009): 178-181

Topological superconductor



Science 346.6209 (2014): 602-607

Nodal line semimetals

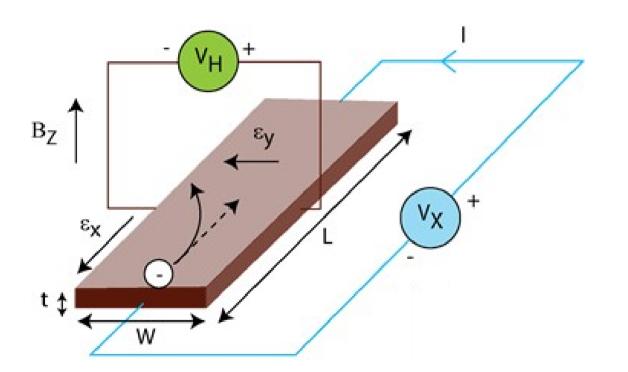


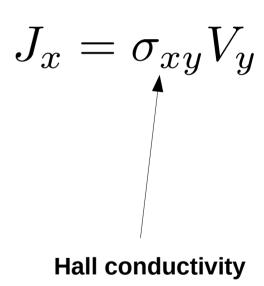
 Mg_3Bi_2

Advanced Science 6.4 (2019): 1800897

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

The Hall effect





Measure the current perpendicular to a voltage

The Hall conductivity

The Hall conductivity is obtained as
$$\sigma_{xy} = \sum_{lpha \in occ} \int \Omega_{lpha} d^2 {f k}$$

Berry curvature

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

Berry connection

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

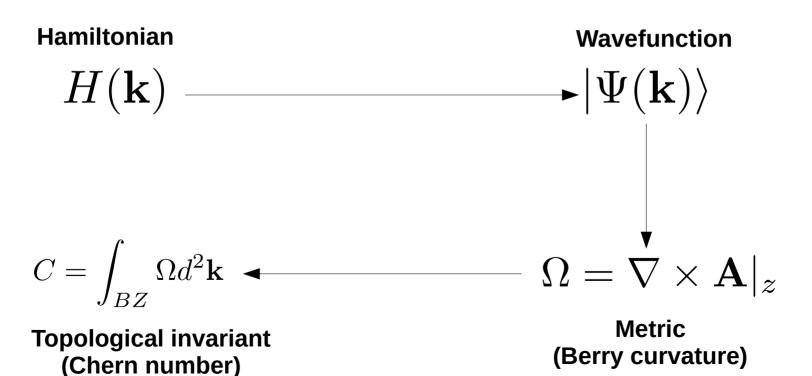
$$\sigma_{xy} = \sum_{\alpha \in occ} \int \Omega_\alpha d^2 \mathbf{k} = \sum_\alpha C_\alpha = C \blacktriangleleft \text{ Chern number}$$

The transverse conductivity is a topological invariant

This means, it must take integer values regardless of defects in an insulator

Topological invariant in a Hamiltonian

We can classify Hamiltonians according to topological invariants



The role of a topological invariant

Hamiltonians with different topological invariants can not be deformed one to another

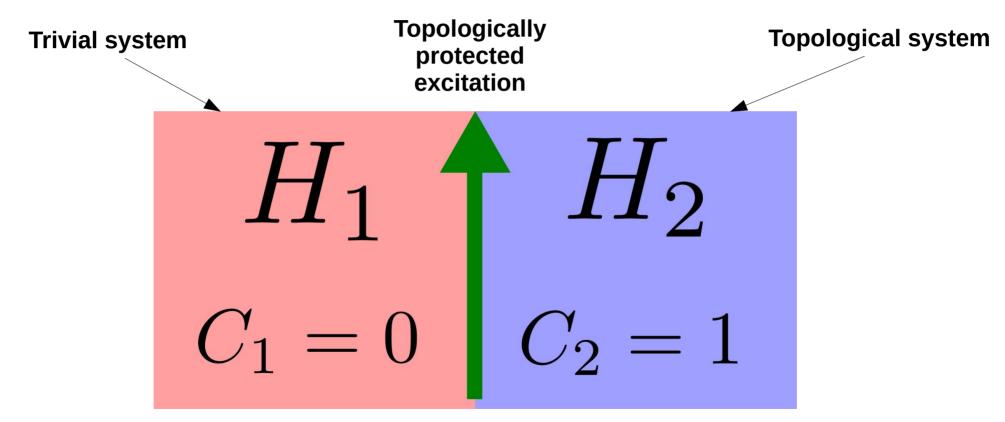
$$C=1$$

$$C=2$$





The consequence of different topological invariants



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

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

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

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

Kernel polynomial for topological invariants in real-space

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

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

With a kernel polynomial tensor network algorithm

$$\hat{\mathcal{P}} = \sum_{n} T_n(\hat{\mathcal{H}}) \int_{-\infty}^{\varepsilon_F} d\omega \frac{T_n(\omega)}{\sqrt{1 - \omega^2}}, \qquad T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x)$$
$$T_0 = 1 \text{ and } T_1(x) = x$$

Phys. Rev. B 84, 241106® (2011)

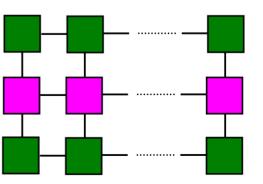
Computing Chern numbers with tensor networks

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

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



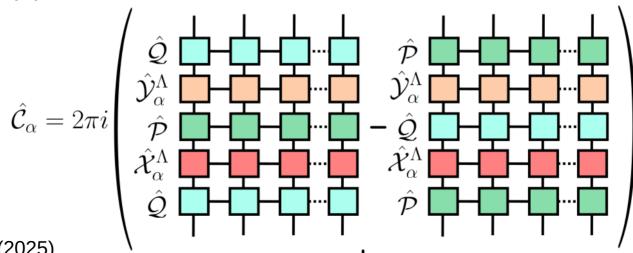
arXiv:2506.05230 (2025)

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



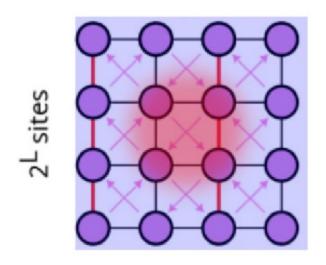
arXiv:2506.05230 (2025)

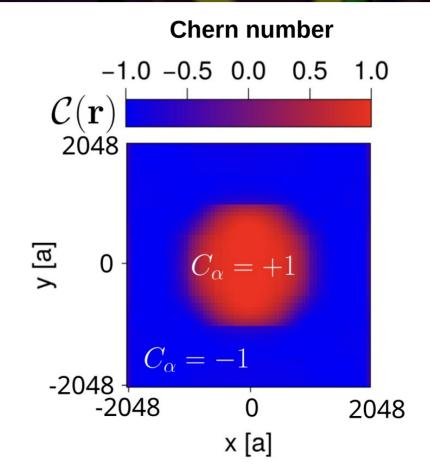
Topological domain with tensor networks

arXiv:2506.05230 (2025) **Topological marker**

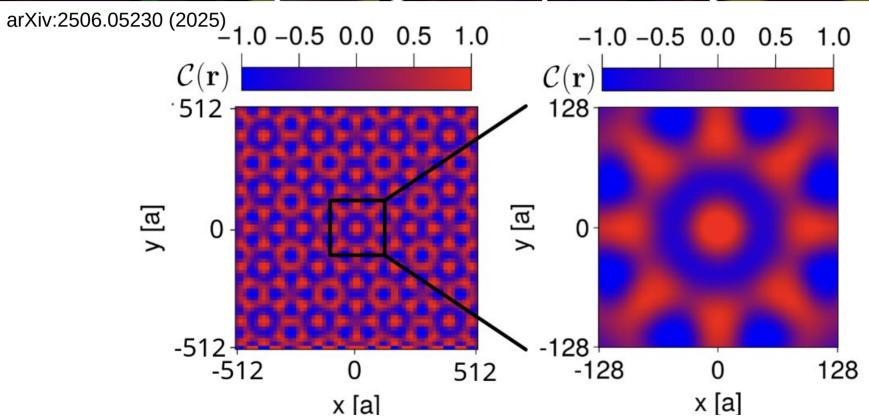
$$C_{\alpha} = 2\pi i \langle \alpha | \hat{Q}\hat{X}\hat{P}\hat{Y}\hat{Q} - \hat{P}\hat{X}\hat{Q}\hat{Y}\hat{P} | \alpha \rangle$$

In a spatially modulated topological Hamiltonian



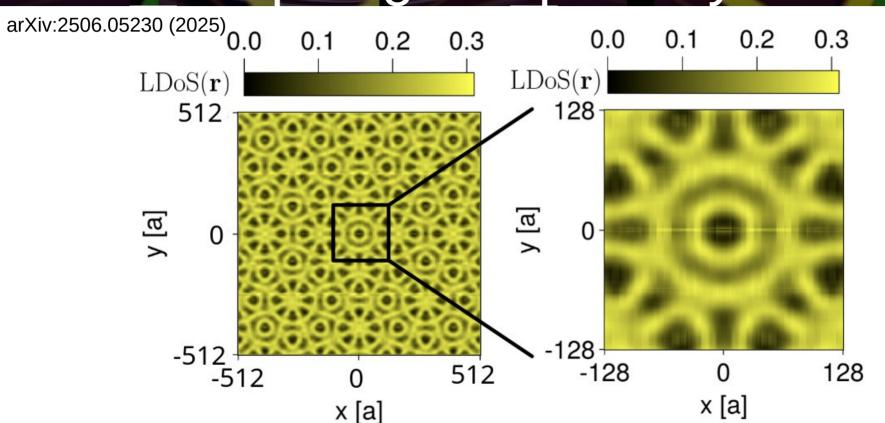


Chern mosaic in a 8-fold topological quasicrystal



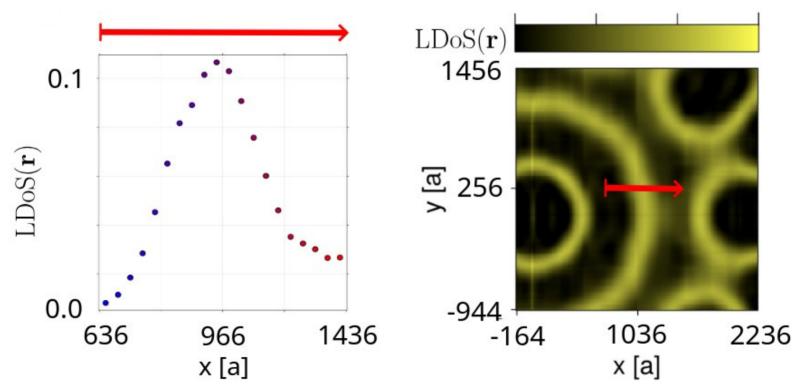
Domains with different topological invariants can be directly computed in real space

Topological modes in a 8-fold topological quasicrystal



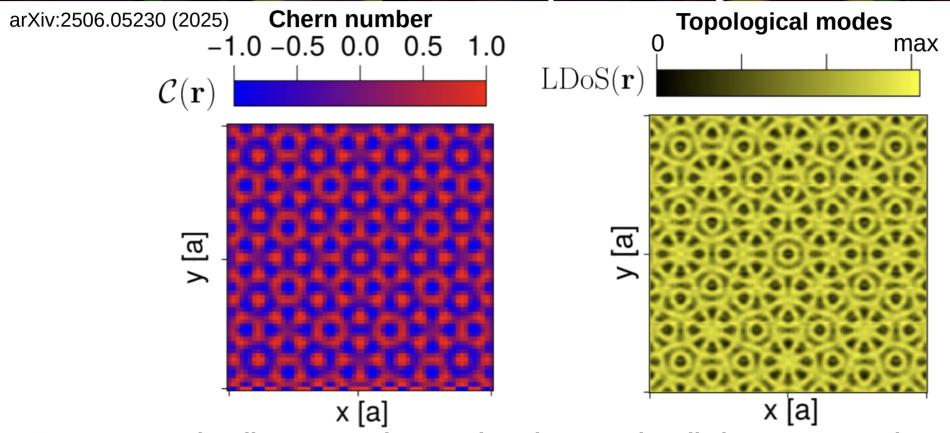
Topological modes appear between topological domains in real space

Zero modes across topological quasicrystalline domain



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

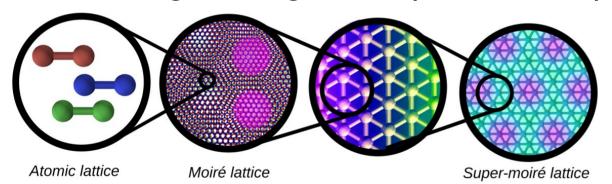
Chern mosaic and topological modes in a quasicrystal



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

Summary

Tensor networks allows solving large electronic structure problems, reaching the regime required for super-moire materials



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

$$\mathcal{H}_{\alpha\beta}^{MF} \equiv \begin{array}{c} & \\ \\ \end{array} = \begin{array}{c} \\ \end{array} =$$

$$\hat{C}_{\alpha} = 2\pi i \begin{pmatrix} \hat{\mathcal{Q}} & & & & \\ \hat{\mathcal{Y}}_{\alpha}^{\Lambda} & & & & \\ \hat{\mathcal{Y}}_{\alpha}^{\Lambda} & & & & \\ \hat{\mathcal{P}} & & & & \\ \hat{\mathcal{Z}}_{\alpha}^{\Lambda} & & & & \\ \hat{\mathcal{Q}} & & & & & \\ \hat{\mathcal{Q}} & & & & & \\ \hat{\mathcal{Q}} & & & & & \\ \end{pmatrix}$$