Solving single-particle matter above one trillion sites with quantum many-body tensor network algorithms

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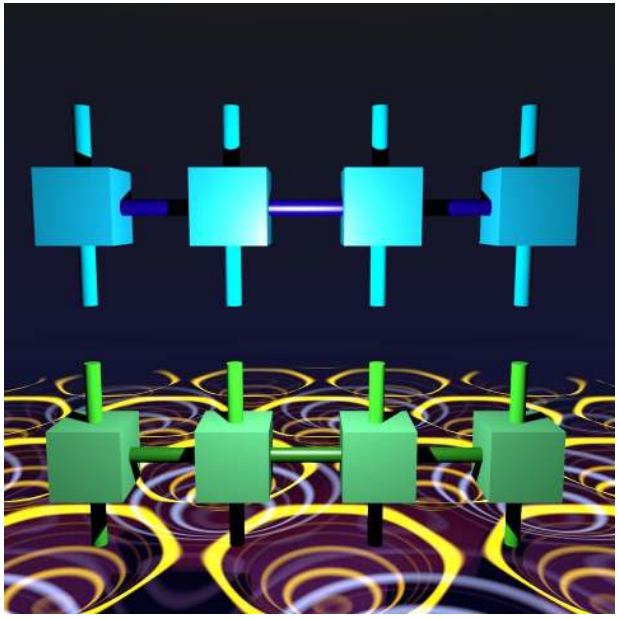
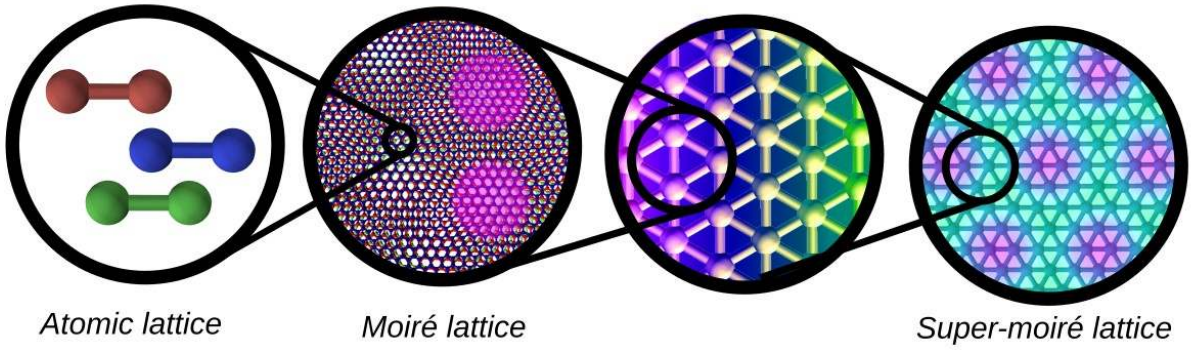
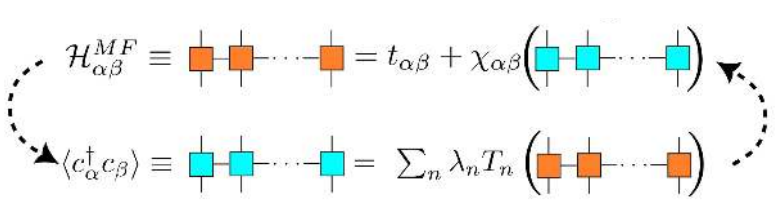
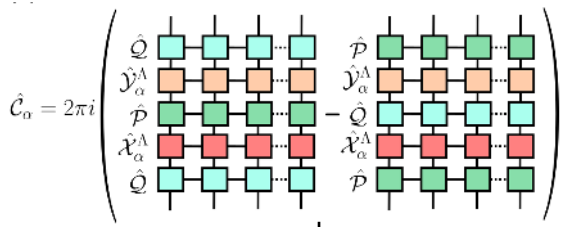








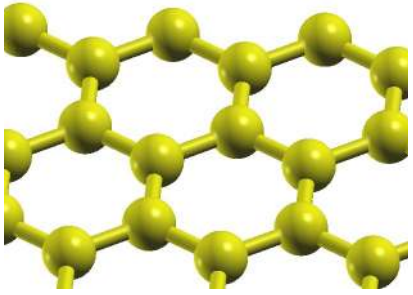
arXiv:2507.04262 (2025) *arXiv:2506.05230 (2025)* *arXiv:2503.04373 (2025)*

Nordic Quantum Information Processing workshop, Nordita, Sweden, November 26th 2025

The two-dimensional materials world

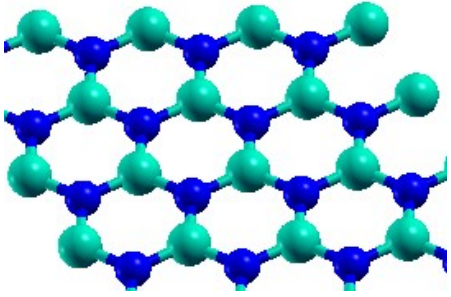
Semimetal

Graphene



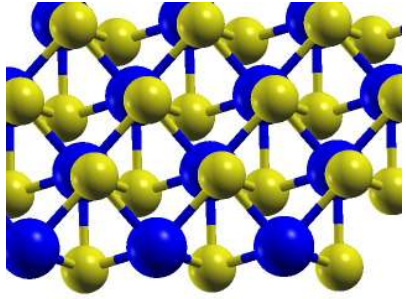
Insulator

BN



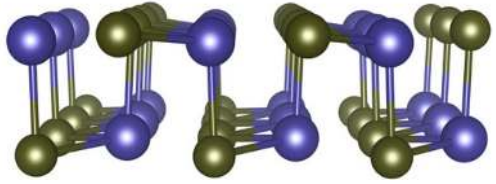
Superconductor

$NbSe_2$



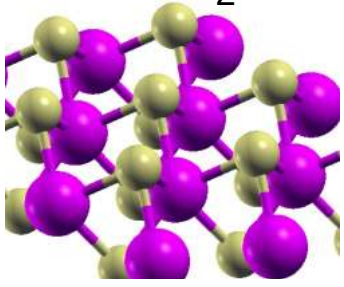
Ferroelectric

SnTe



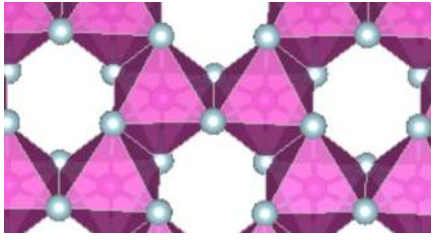
Semiconductor

WS_2



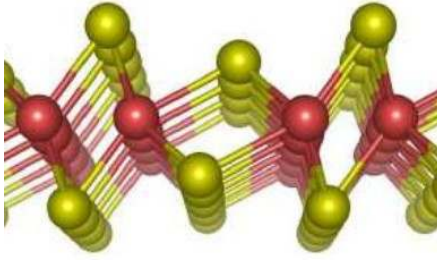
Ferromagnet

CrI_3



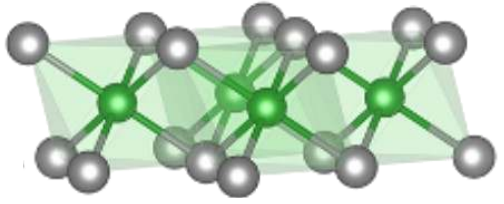
Quantum spin Hall insulator

WTe_2



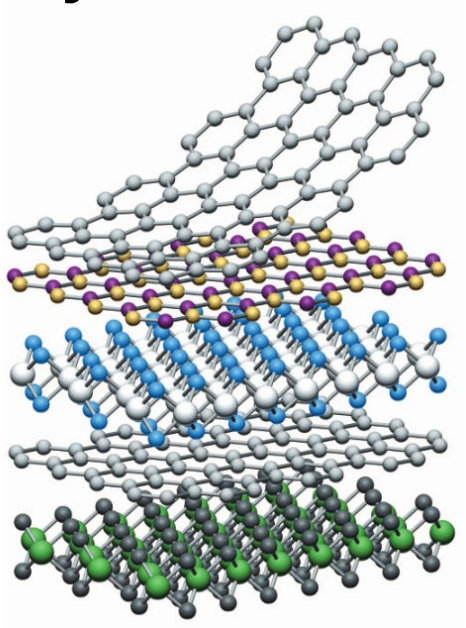
Multiferroic

NiI_2



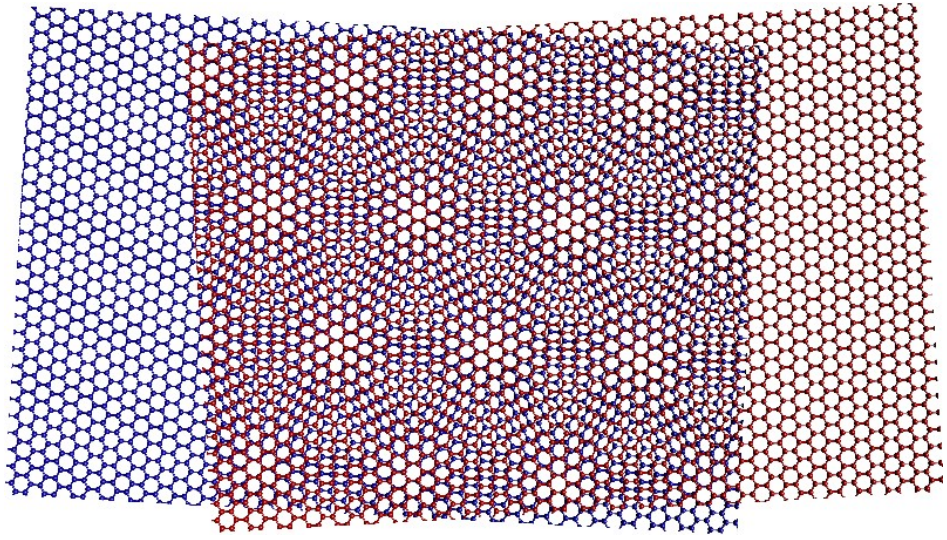
The flexibility of two-dimensional materials

They can be stacked



Nature 499, 419–425 (2013)

They can be rotated

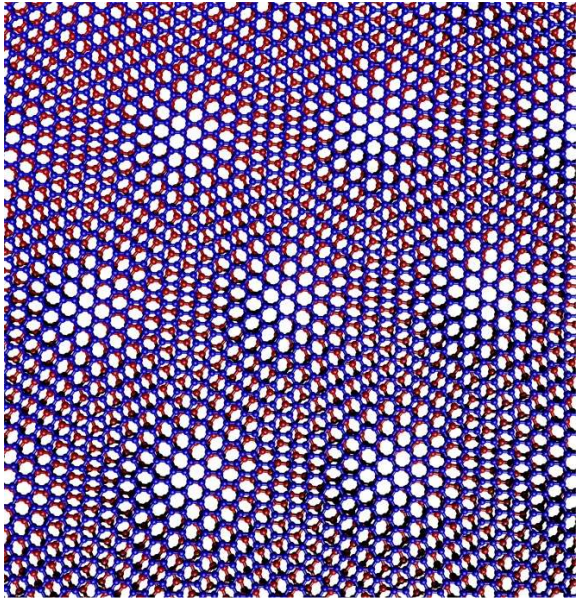


Science 361, 6403, 690-693 (2018)

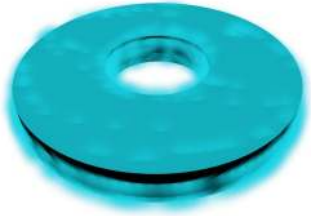
These are unique features of two-dimensional materials

The tunability of twisted van der Waals materials

Twisted bilayer graphene



Superconductivity

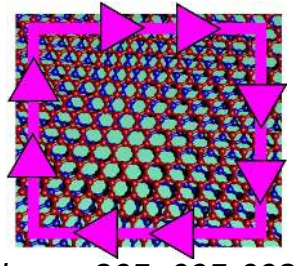


Nature 556, 43–50 (2018)

Topological networks

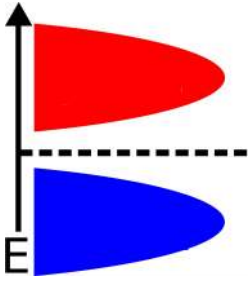
Nano Lett. 18, 11, 6725-6730 (2018)

Chern insulators



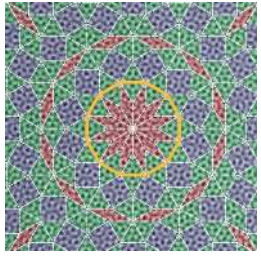
Science 365, 605-608 (2019)

Correlated insulators



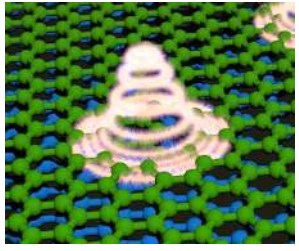
Nature 556, 80–84 (2018)

Quasicrystalline physics



Science 361, 782-786 (2018)

Proximal fractional Chern insulators

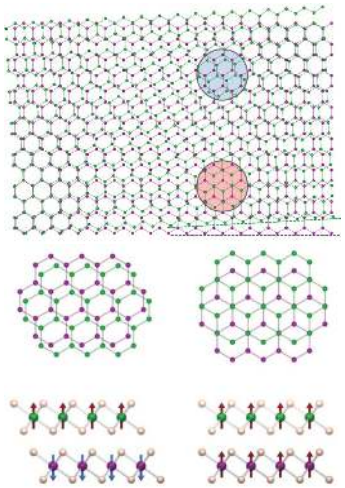


Nature 600, 439–443 (2021)

Twisted multilayers provide a powerful platform for emergent phenomena

Artificial quantum matter in moire van der Waals heterostructures

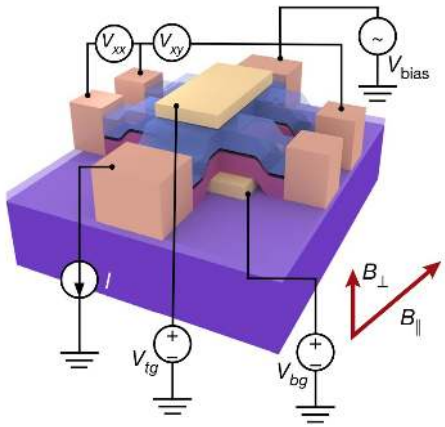
Unconventional magnets



Twisted $CrBr_3$

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

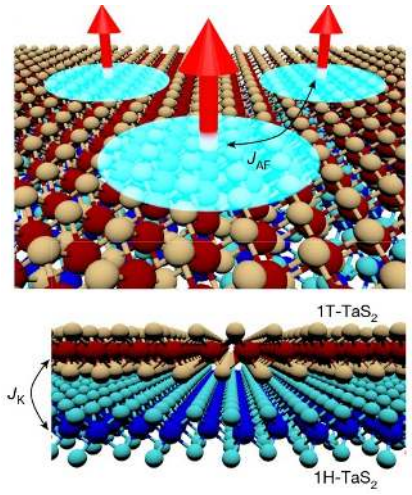
Unconventional superconductors



Twisted trilayer graphene

Nature 595, 526–531 (2021)

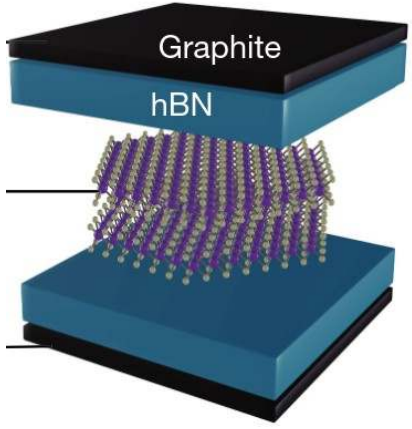
Heavy-fermion quantum materials



1H-1T TaS_2

Nature 599, 582–586 (2021)

Fractional topological matter

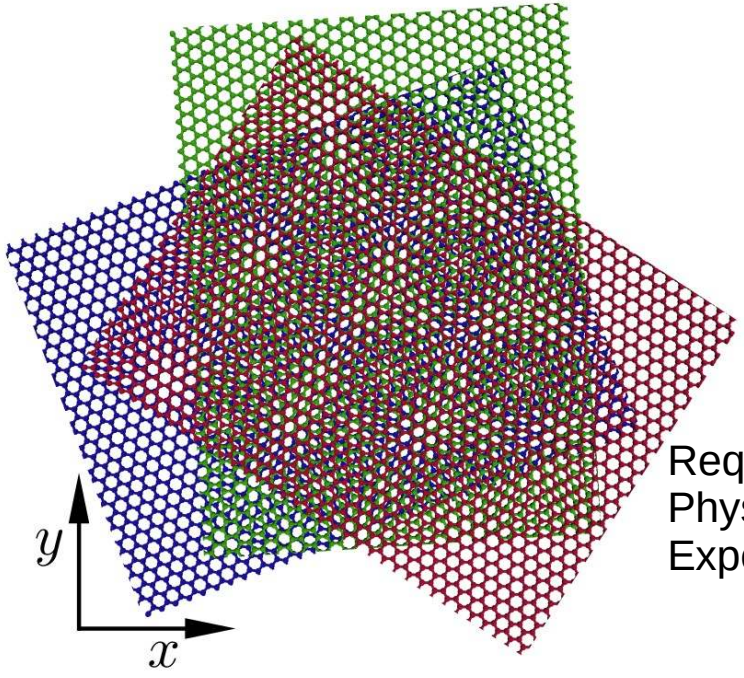


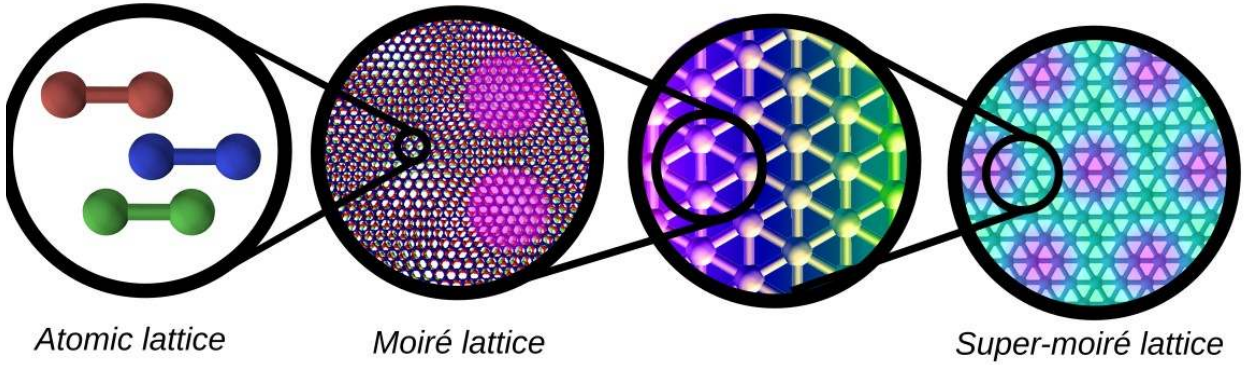
Twisted $MoTe_2$

Nature 622, 63–68 (2023)

Super-moire materials

Moire-of-moire materials



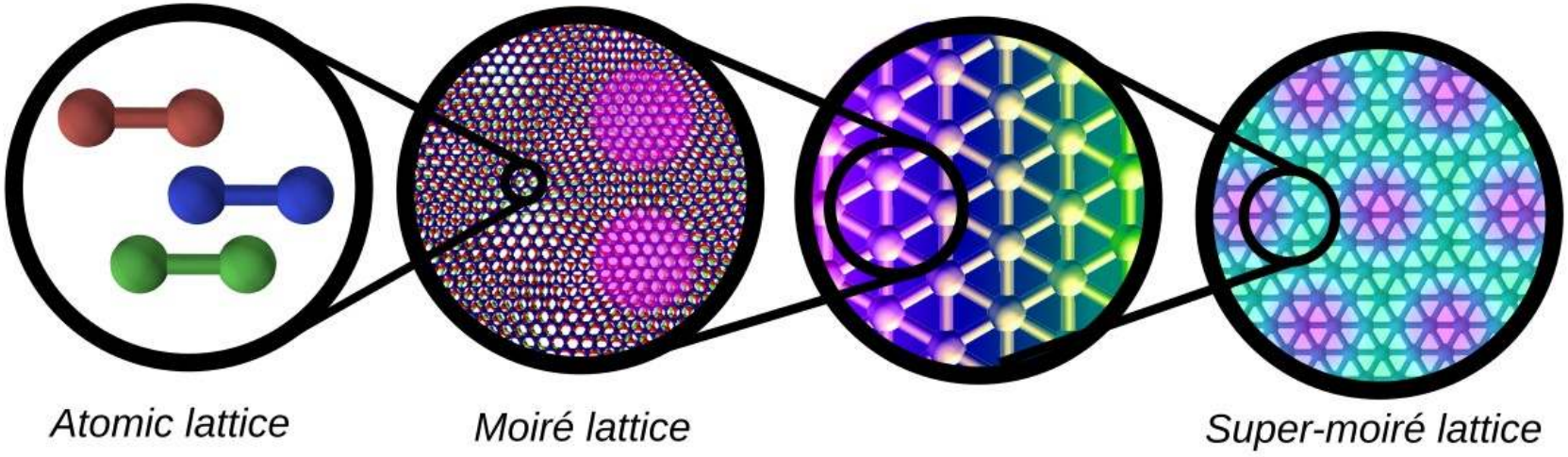


Requires computing up to a billion sites (10^9)
Physics at several length scales (atomic, moire, and super-moire)
Experiments showing correlations and unconventional superconductivity

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

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

Why super-moire materials are hard (for theorists)



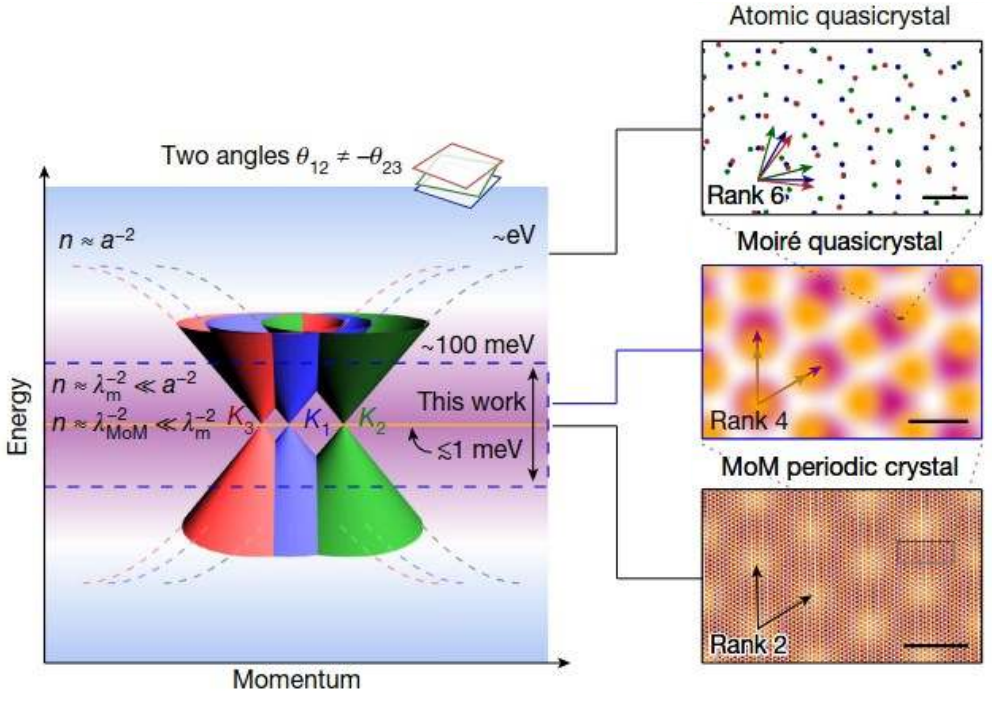
Moire systems **N=10^5 sites**, calculations taking around 1 minute
Computational cost grows as **N** (best case) or **N^3** (worst case)
Super-moire **N=10^9 sites**, calculations taking 10 days – 1000000 years

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

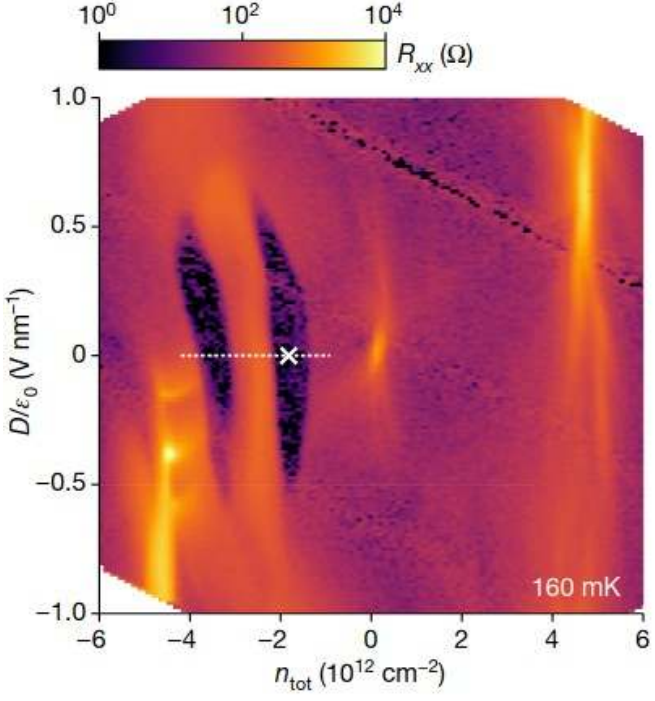
(even going beyond usual memory limitations of conventional methods)

Super-moire materials, experimentally

Moire quasicrystal in twisted trilayer graphene



Coexisting correlations and superconductivity



Nature 620, 762–767 (2023)

Behind the scenes

Yitao Sun

Tiago Antão

Marcel Niedermeier

Adolfo Fumega

Adrien Moulinas

Thibaud Louvet

Xavier Waintal

Solving the Gross-Pitaevskii equation on multiple different scales using the quantics tensor train representation, M. Niedermeier, A. Moulinas, T. Louvet, J. L. Lado, X. Waintal, **arXiv:2507.04262 (2025)**

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, **arXiv:2503.04373 (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)**

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

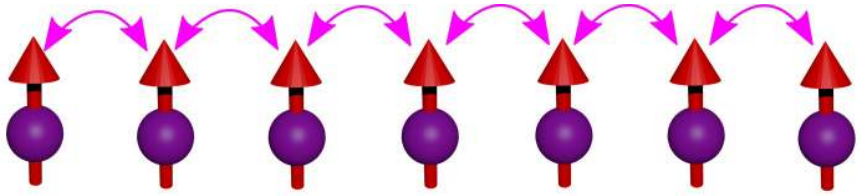
The problem of dimensionality

In a many-body problem, the size of our vectors grows as

$$2^L$$

where L is the number of sites

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



For a single-particle tight binding problem, we can reach up to 10^8 sites in a laptop

For a many-problem, we cannot even store states for systems bigger than $L = 30$ sites

$$2^{30} \sim 10^9$$

The quantum many-body problem

Let us take a simple many-body problem

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

A typical wavefunction is written as

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

We need to determine in total 2^L coefficients

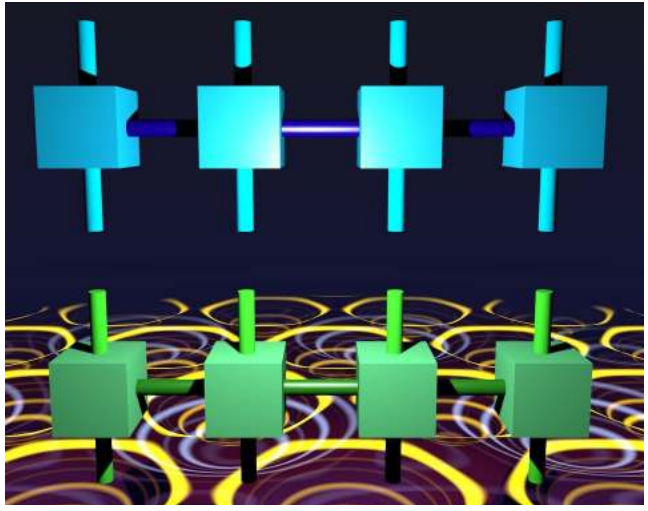
Is there an efficient way of storing so many coefficients?

Dealing with very large spaces with tensor networks

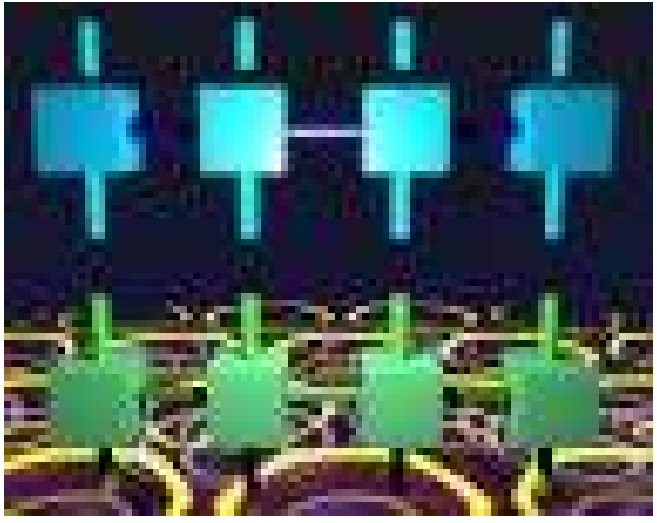
A many-body wavefunction a is a very high dimensional object (2^L coefficients)

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

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



“True wavefunction”



“Tensor-network wavefunction”

Dealing with very large spaces with tensor networks

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

Tensor networks allow parametrizing many-body wavefunctions as

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

$L\chi^2$ parameters

Full wavefunction  *Matrix product state*

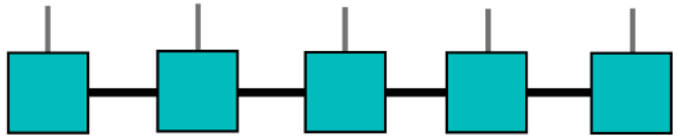
Tensor networks allow to drastically reduce the memory required to store a many-body state

Annals of Physics 326, 96 (2011)

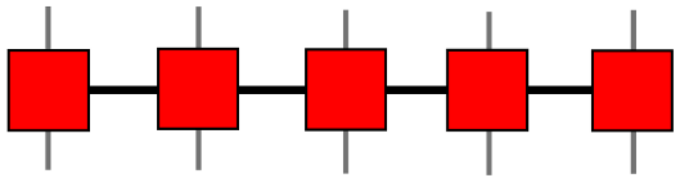
Exponentially large algebra with tensor networks

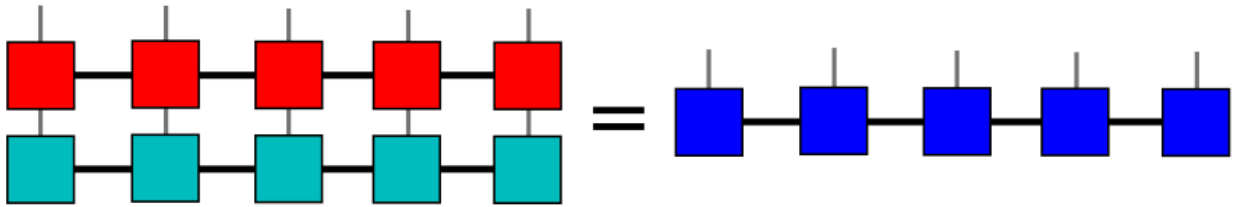
Tensor network allow to (approximately) operate in exponentially large vector spaces

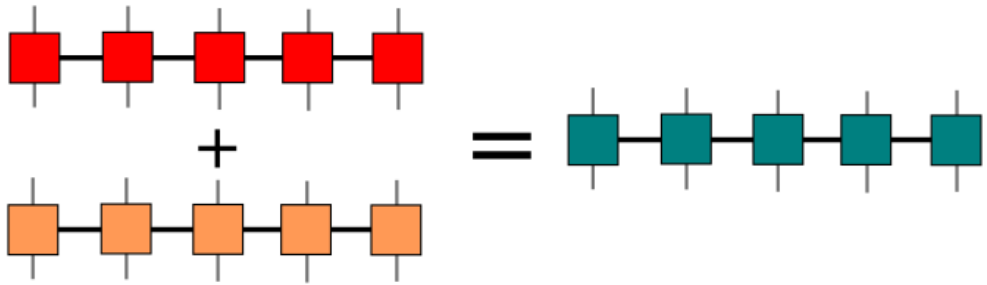
vector

$|\Psi\rangle \equiv$ 

matrix

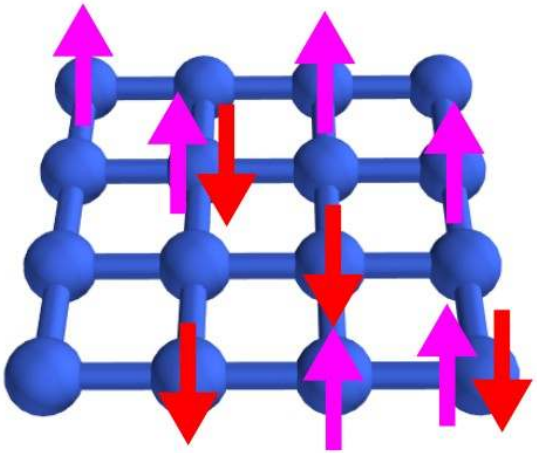
$\hat{A} \equiv$ 

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

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

Some paradigmatic problems solved with matrix product states

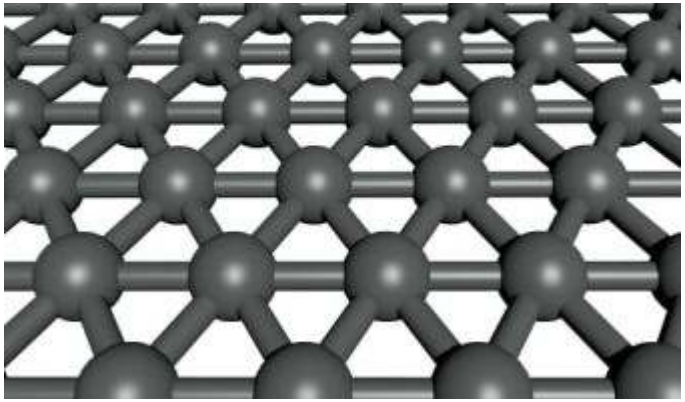
Solving the 2D Hubbard model at finite doping



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

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

Solving the 2D Heisenberg model in frustrated lattices

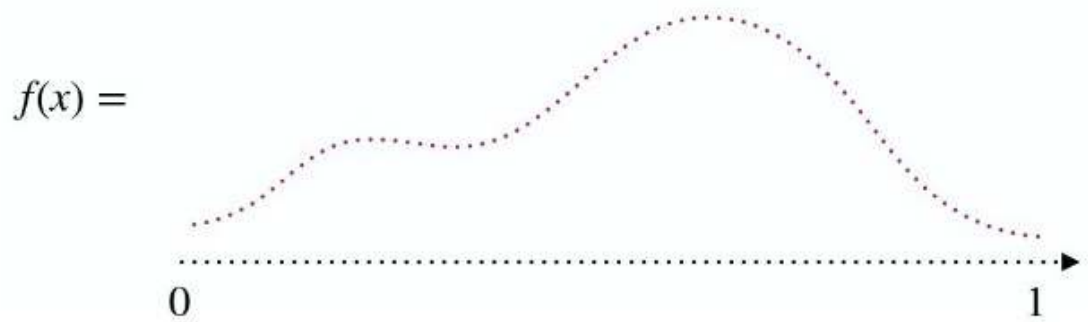


$$\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

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

Tensor networks for non quantum-many body

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



We could store all those values with a tensor network

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

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

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

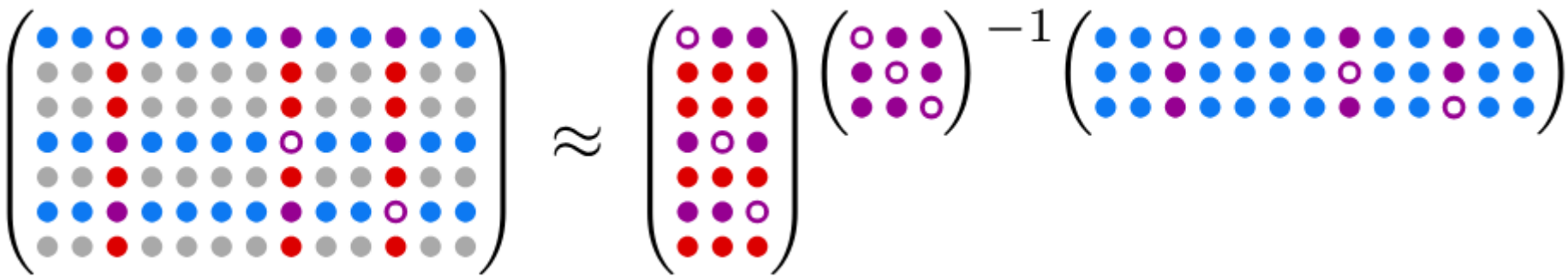
Quantum-inspired active learning algorithm

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

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



Quantum inspired active learning to learn exponentially large spaces

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

SciPost Phys. 18, 104 (2025)

Tensor networks for non-linear time-dependent differential equations

Non-linear time-dependent differential equation

The Gross-Pitaevskii equation

$$i\frac{\partial\psi}{\partial t} = \left[-\frac{1}{2m}\hat{\nabla}^2 + \hat{V} + g|\psi|^2\right]\psi$$

In a complex potential

$$\hat{V}(x,y) = A_x\left(\frac{x}{W}\right)^2 + A_y\left(\frac{y}{W}\right)^2 + A_{xy}\frac{xy}{W^2} + A\sum_i \sin^2(\boldsymbol{q_i}\cdot\boldsymbol{r}),$$

Tensor network decomposition of the solution

$$\psi(\sigma_R\sigma_{R-1}...\sigma_1) \approx M^{i_{R-1}}_{\sigma_R} M^{i_{R-1}i_{R-2}}_{\sigma_{R-1}} ... M^{i_1}_{\sigma_1}$$

Discretization

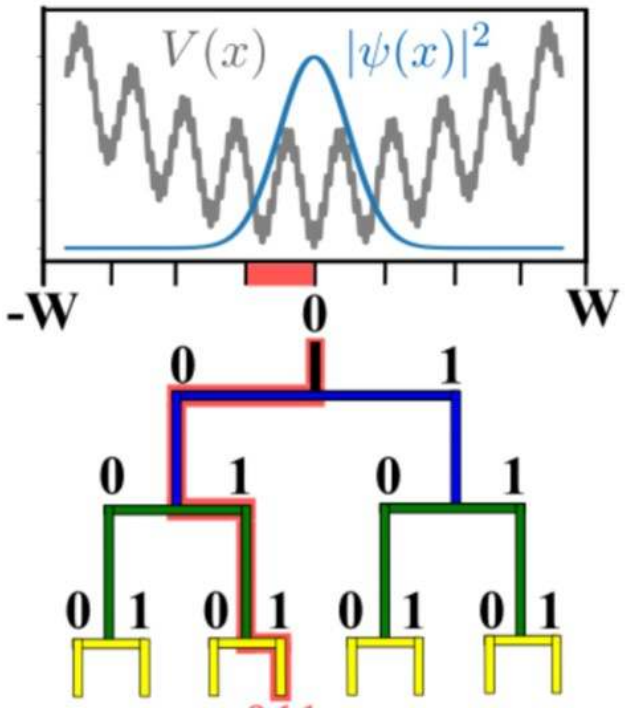
$$x(m) = -W + mh_r$$

Quantics representation

$$m = \sum_{i=1}^{R}\sigma_i 2^i \equiv (\sigma_R\sigma_{R-1}...\sigma_1)$$

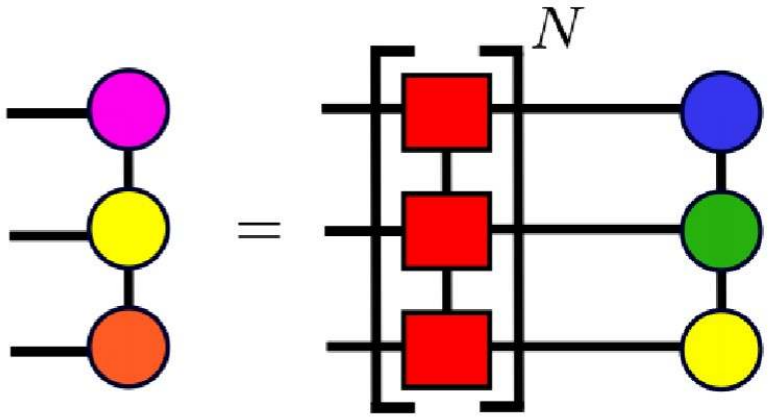
Solving the Gross-Pitaevskii equation with tensor networks

Quantics representation



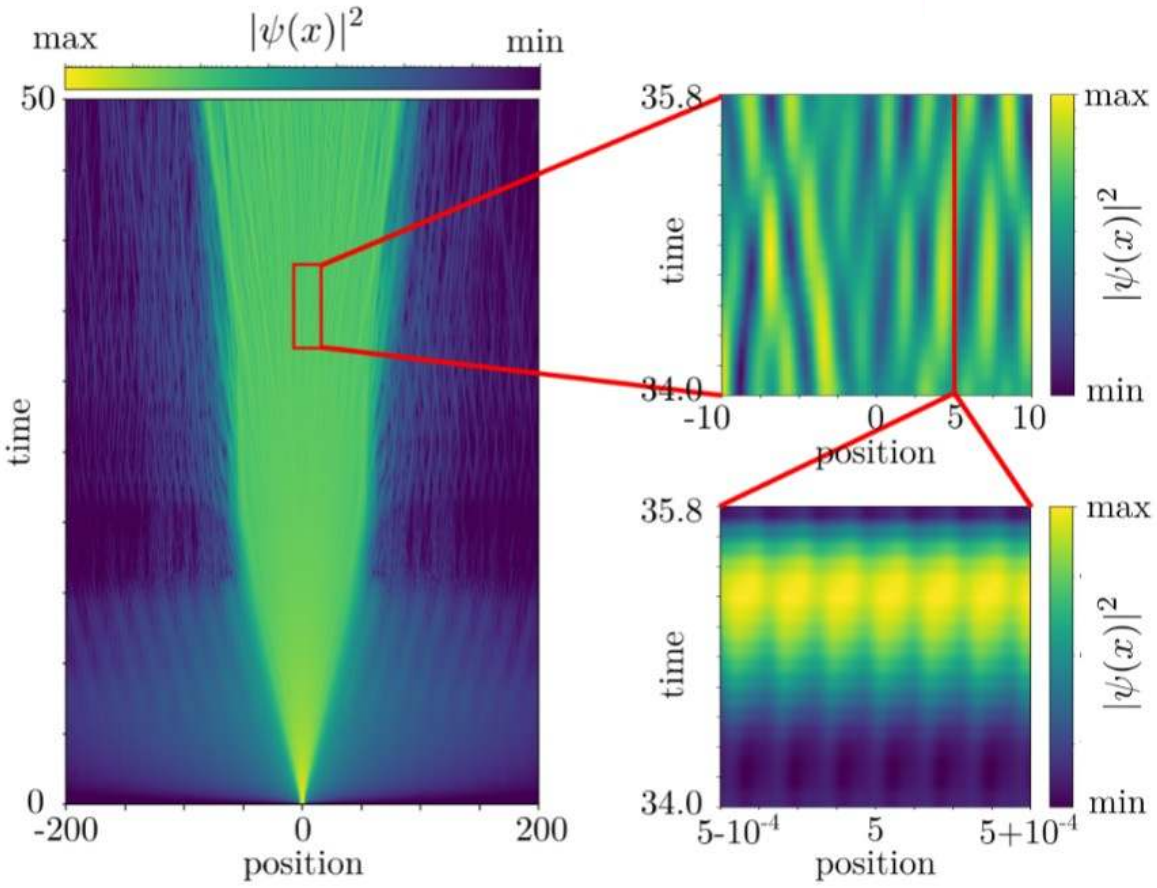
Tensor-network evolution

$$|\psi(Nh_t)\rangle = \left[\hat{U}(h_t)\right]^N |\psi_0\rangle$$



arXiv:2507.04262 (2025)

Gross-Pitaevskii evolution in highly features microscopic potentials



Two length scales

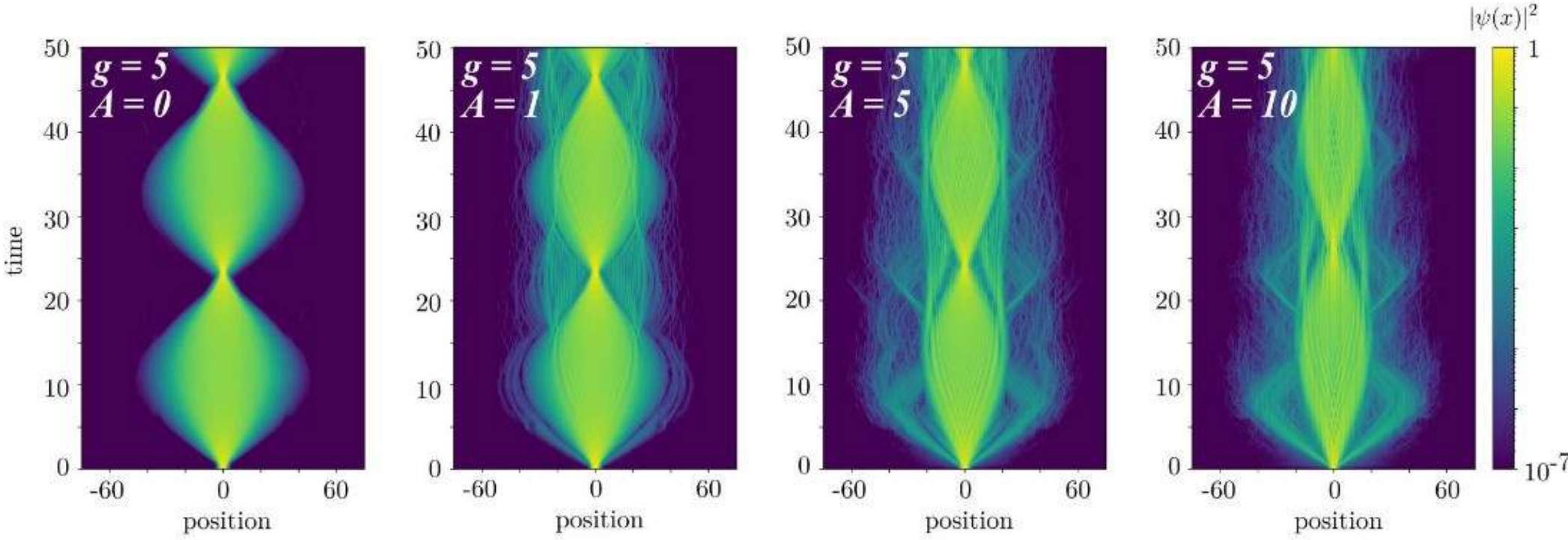
Large-scale harmonic trap

Short-scale moire potential

arXiv:2507.04262 (2025)

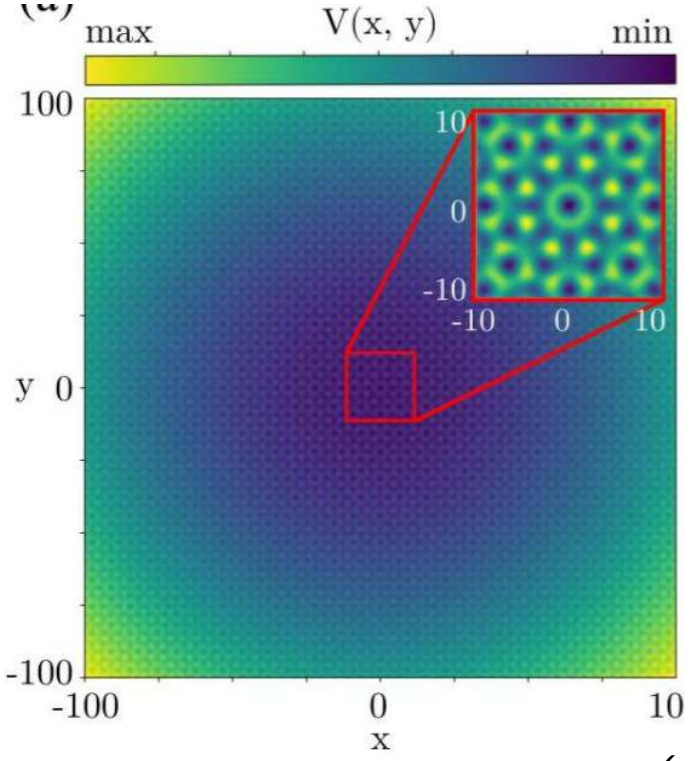
One-dimensional harmonic-moire potential

Tensor networks allow solving the dynamics in a potential with widely different length scales

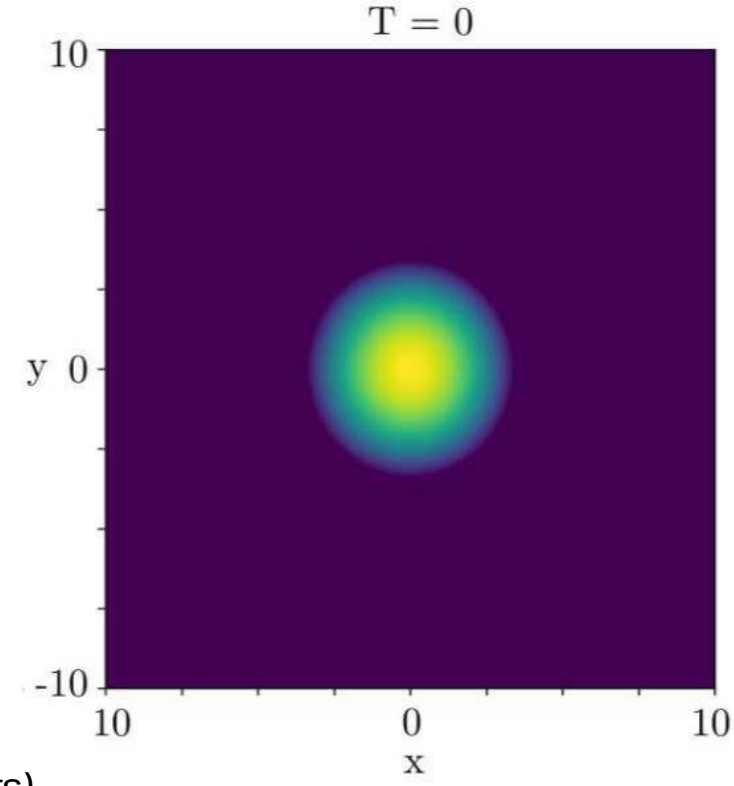


Two-dimensional Gross-Pitaevskii in a quasicrystalline potential

Eight-fold symmetric potential



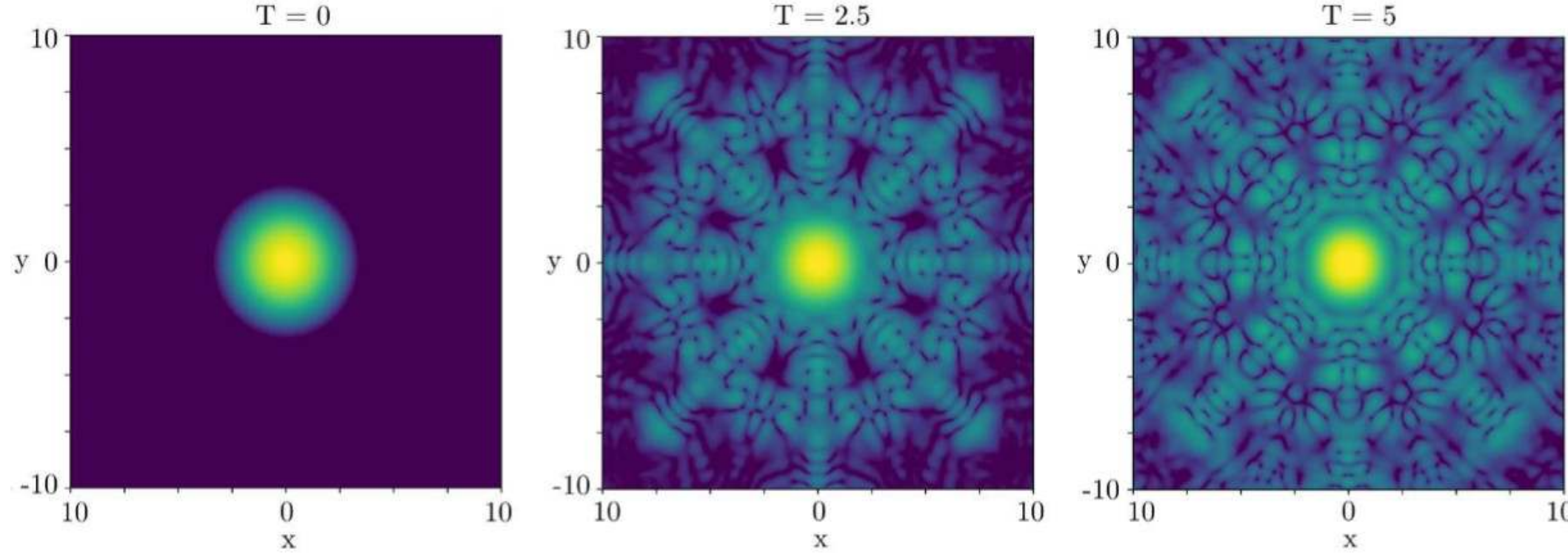
Initial state



(with a trillion grid points)

Two-dimensional Gross-Pitaevskii in a quasicrystalline potential

Tensor network allow computing the evolution with exceptional real-space accuracy



arXiv:2507.04262 (2025)

Tensor networks for interacting super-moire materials

Solving a correlated super-moire material with mean-field

Hamiltonian describing electrons in a super-moire material

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

Mean-field treatment of the interacting Hamiltonian

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

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

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

How could we solve a system whose Hamiltonian would be too large to store?

(even before considering the time required to solve it)

Tensor networks for a super-moire tight binding problem

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

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

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

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

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

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

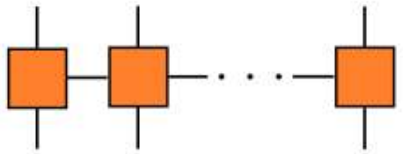
With quantics tensor-cross interpolation: ***a quantum-inspired active learning algorithm***

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

Self-consistent electronic interactions with tensor networks

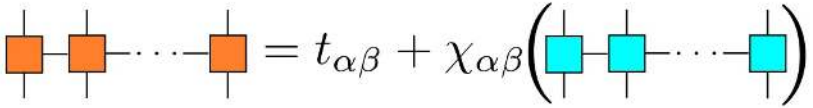
We represent the super-moire electronic Hamiltonian as a tensor-network

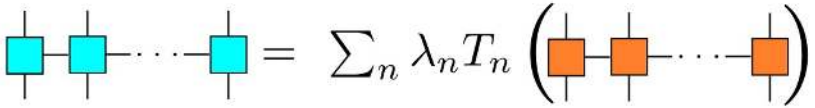
$$\mathcal{H}^{MF}_{\alpha\beta} \equiv \Gamma^{(1)}_{s_1,s_1'}\Gamma^{(2)}_{s_2,s_2'}\Gamma^{(3)}_{s_3,s_3'}...\Gamma^{(L)}_{s_L,s_L'}$$

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

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

Tensor Network SCF loop

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

$\langle c^\dagger_\alpha c_\beta \rangle \equiv$ 

arXiv:2503.04373 (2025)

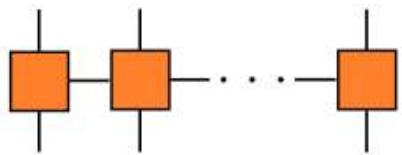
Self-consistent electronic interactions with tensor networks

Super-moire interacting Hamiltonian

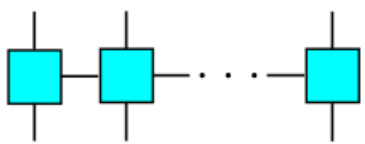
$$H = H_0 + H_V = \sum_{\alpha\beta} t_{\alpha\beta} c_\alpha^\dagger c_\beta + \sum_{\alpha\beta} V_{\alpha\beta} c_\alpha^\dagger c_\alpha c_\beta^\dagger c_\beta$$

Mean-field decoupled Hamiltonian

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

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

Chebyshev expansion of the correlators

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

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

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

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

arXiv:2503.04373 (2025)

Spectral functions with tensor networks

Local spectral function of the mean-field Hamiltonian

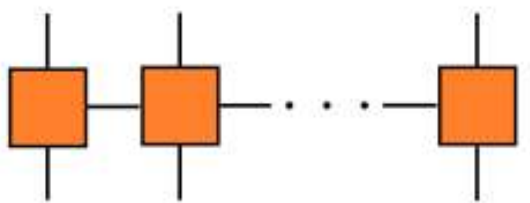
$$D(\omega,\alpha) = \langle\alpha| \left[\sum_n T_n(\mathcal{H}^{MF}) P_n(\omega) \right] |\alpha\rangle$$

With a tensor network Chebyshev algorithm

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

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

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



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

arXiv:2503.04373 (2025)

Tensor network representation of a super-morie Hamiltonian

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

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

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

In the tight binding basis uniform hopping takes the form

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

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

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The tensor-network moire hopping can be built as

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

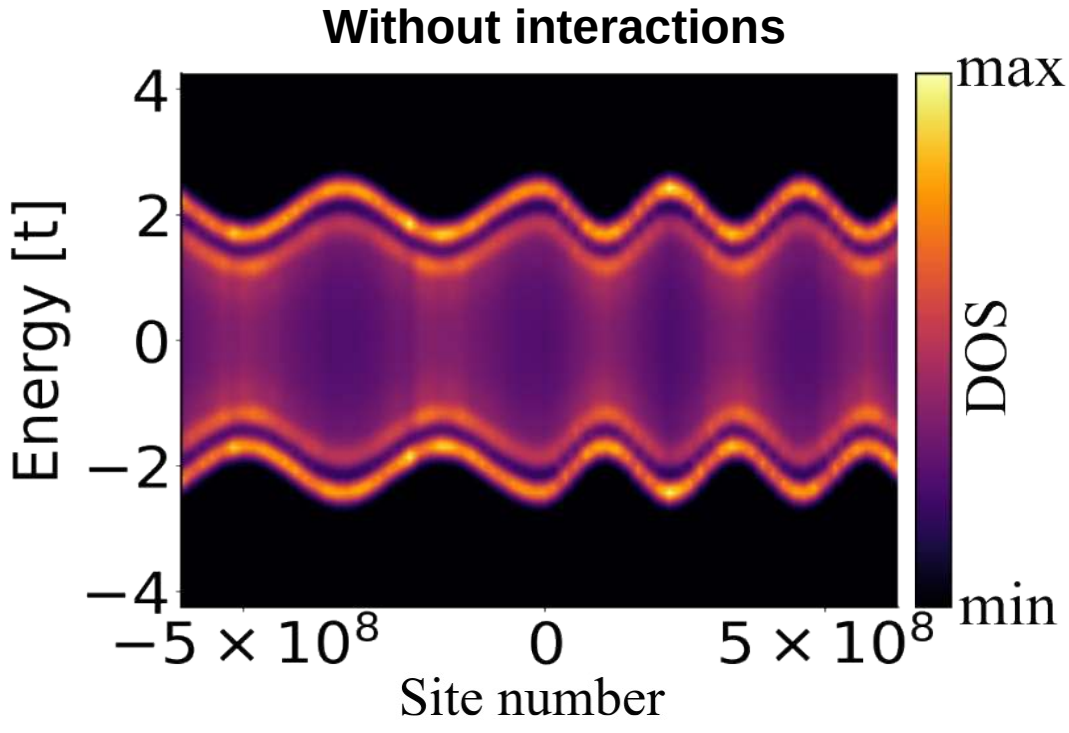
$$|\tau\rangle = \sum M_{s_1}^{(1)} M_{s_2}^{(2)} M_{s_3}^{(3)} ... M_{s_L}^{(L)} \, |s_1, s_2, ..., s_L\rangle$$

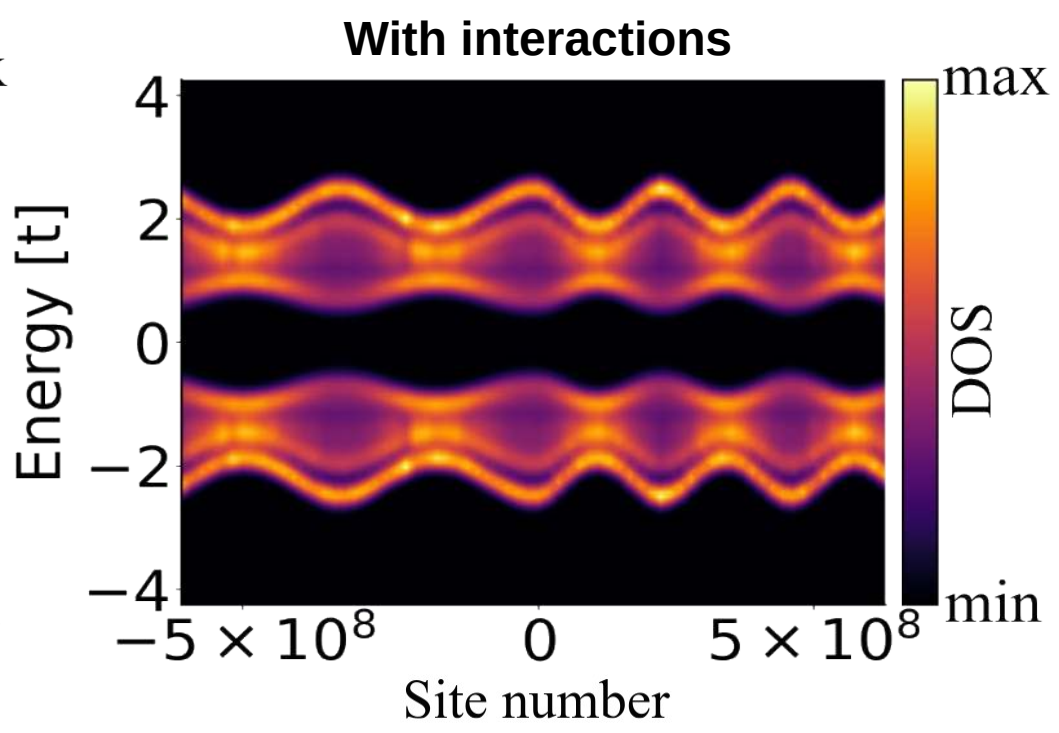
Quantics tensor cross interpolation

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

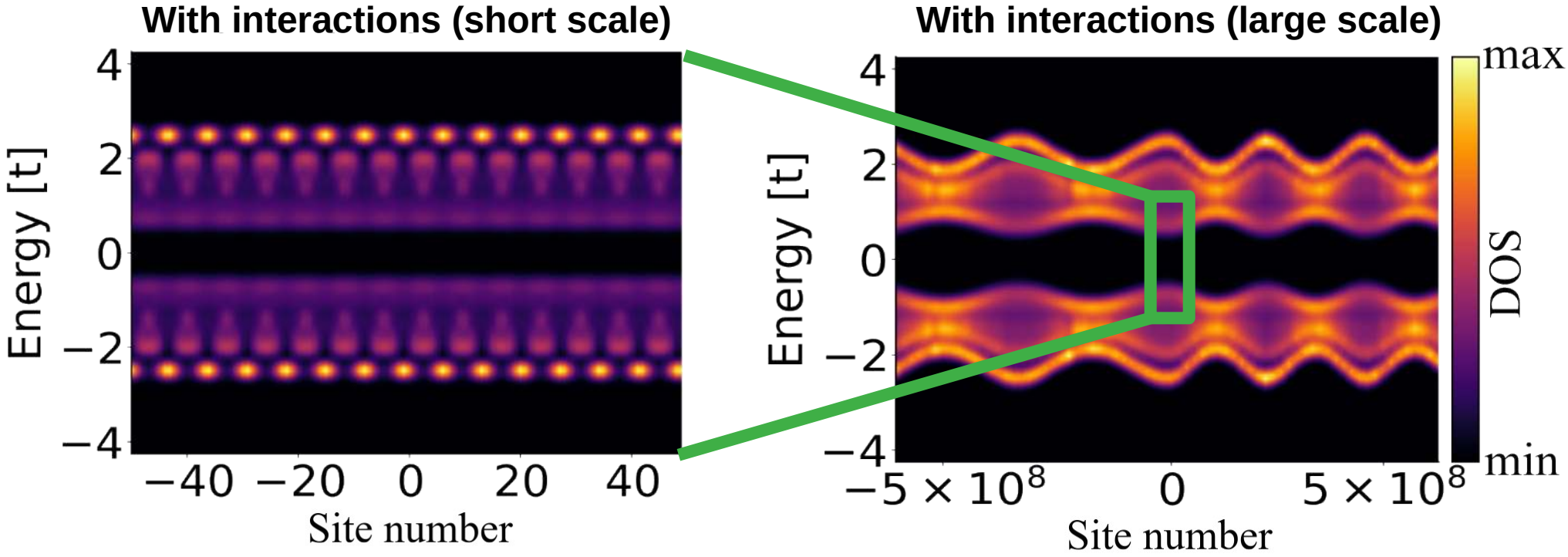




Tensor networks allow to solve selfconsistently a super-moire with one billion sites

arXiv:2503.04373 (2025)

Solving billion-size super-moire materials

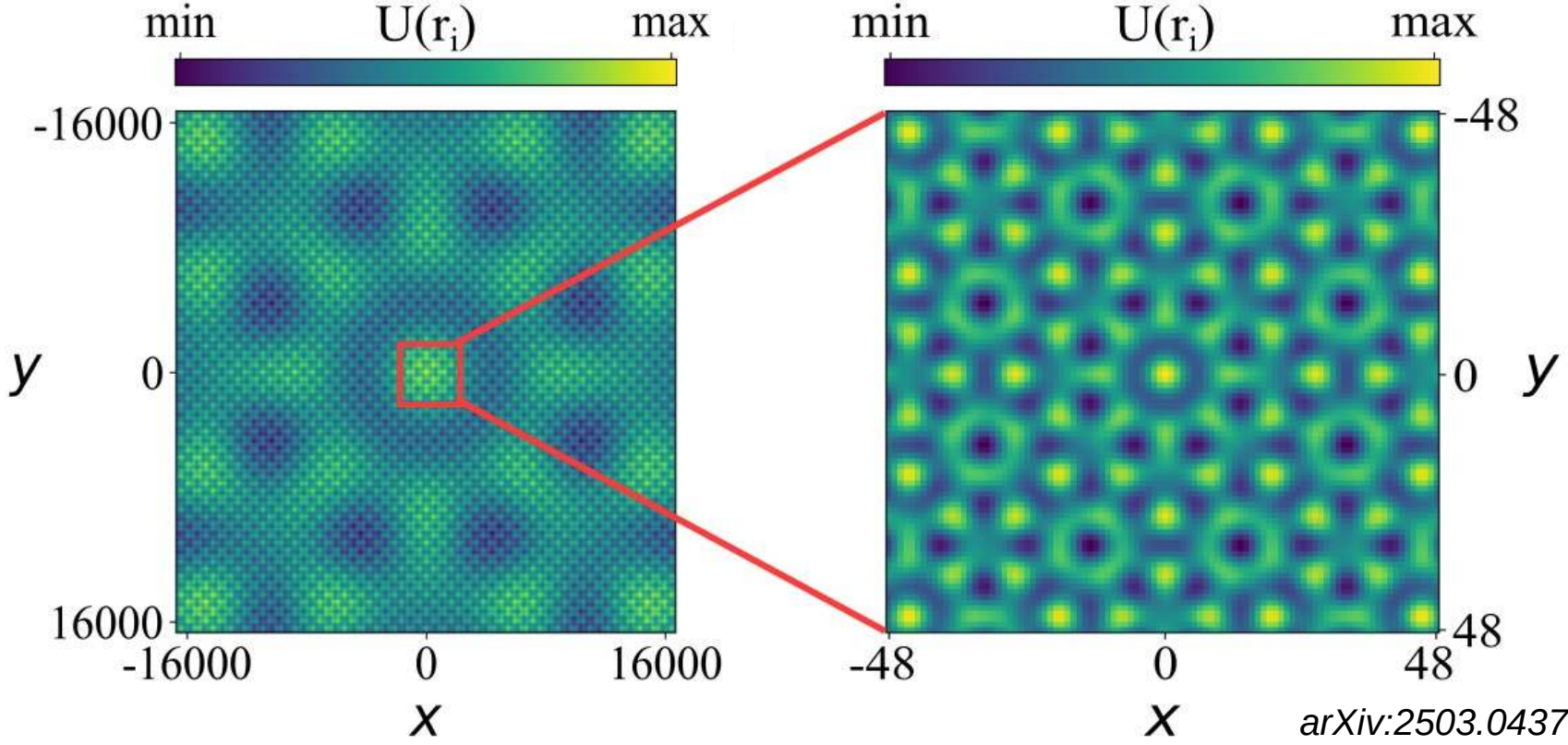


Tensor networks allow to solve selfconsistently a super-moire with one billion sites

arXiv:2503.04373 (2025)

Two-dimensional billion size interacting super-moire

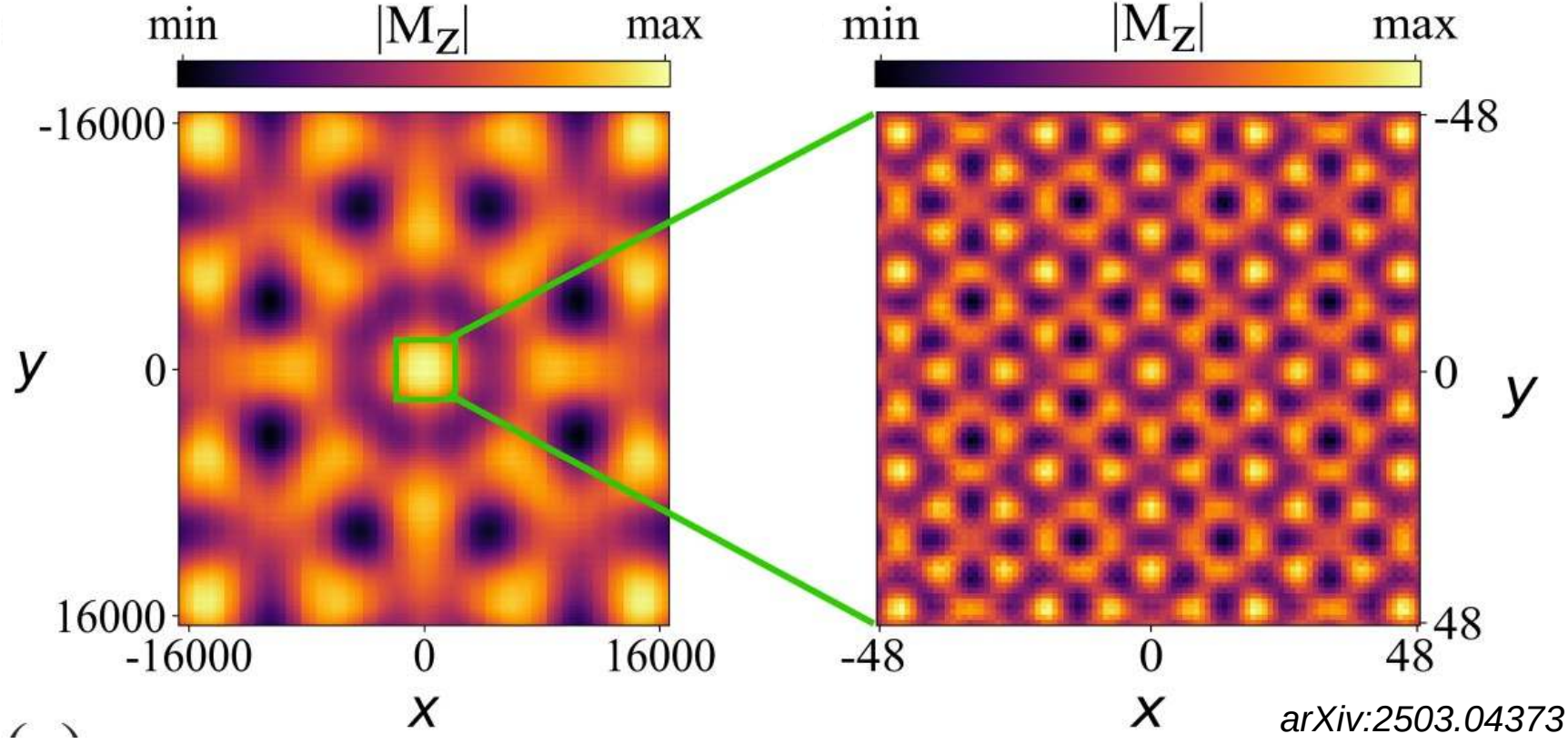
Modulation fo the Hamiltonian



arXiv:2503.04373 (2025)

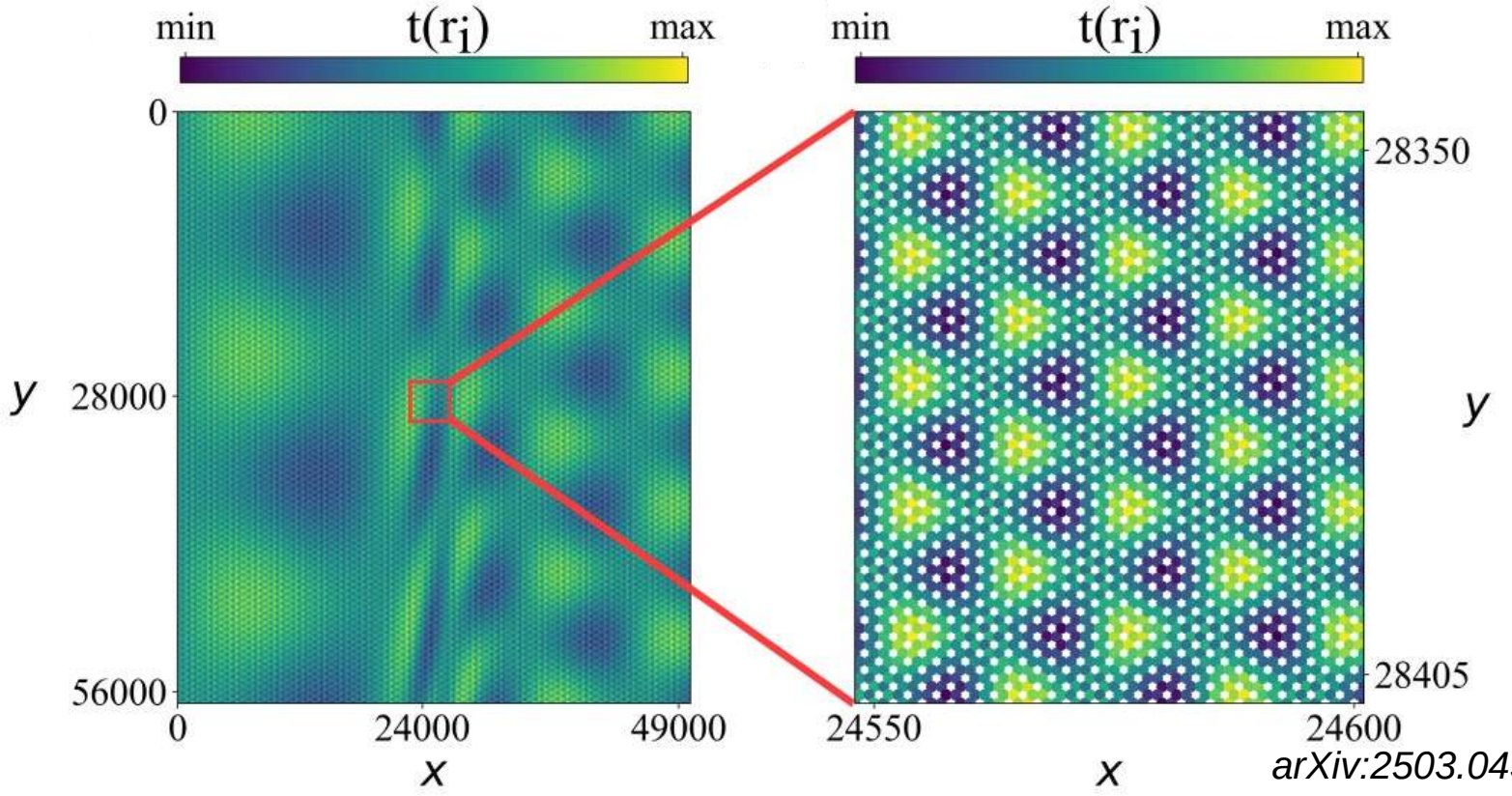
Two-dimensional billion size interacting super-moire

Selfconsistent symmetry broken order (magnetization)



arXiv:2503.04373 (2025)

Two-dimensional billion size interacting super-moire



arXiv:2503.04373 (2025)

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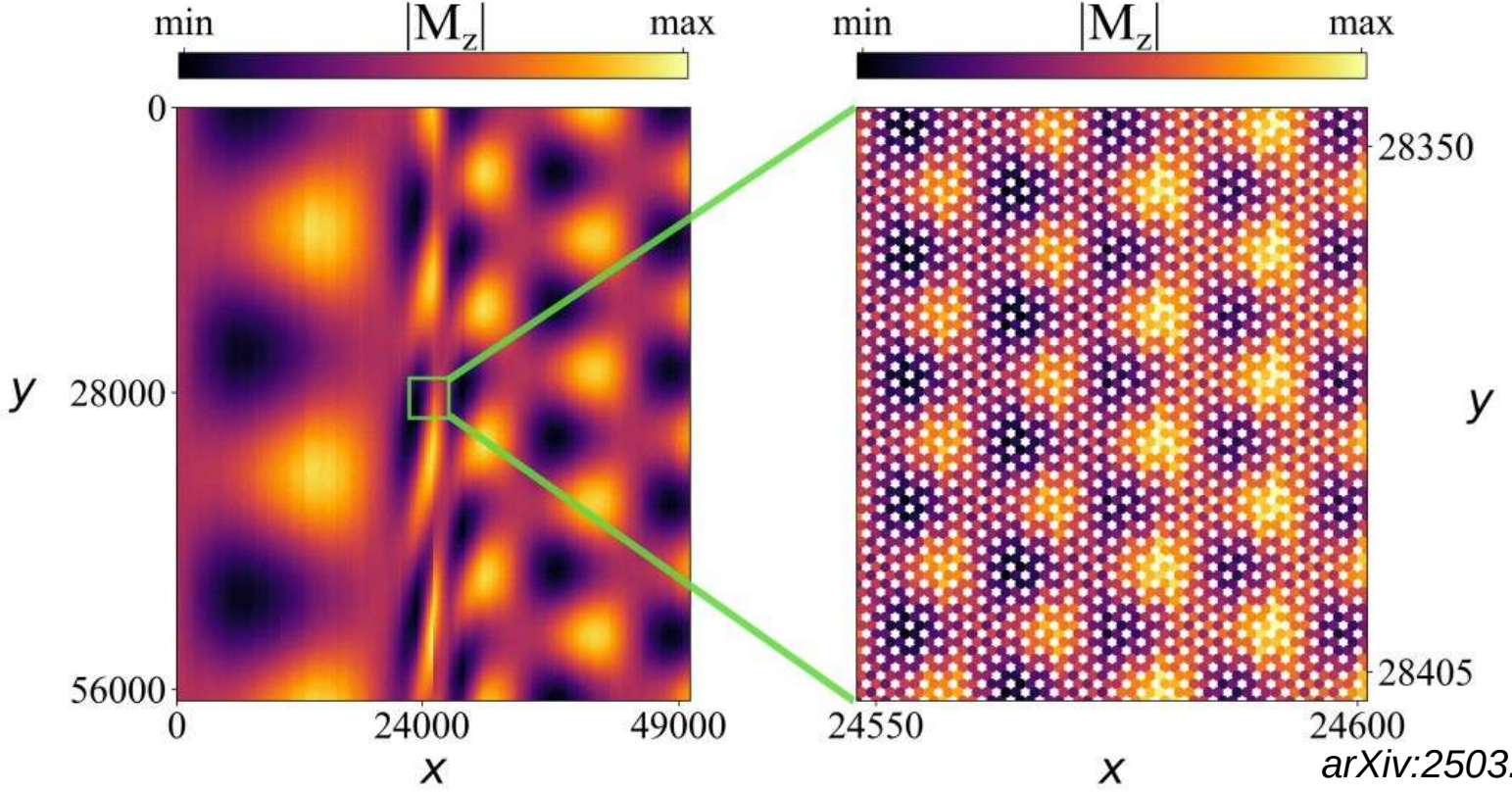


arXiv:2503.04373 (2025)

Tensor networks for topological super-moire materials

Topological invariant in a Hamiltonian

We can classify Hamiltonians according to topological invariants

Hamiltonian $H(\mathbf{k})$ → **Wavefunction** $|\Psi(\mathbf{k})\rangle$

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

Metric (Berry curvature) $\Omega = \nabla \times \mathbf{A}|_z$ → **Topological invariant (Chern number)** $C = \int_{BZ} \Omega d^2\mathbf{k}$

Real space topological invariants

Topological invariants are often defined in reciprocal space

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

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

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

Is it possible to define them in real space?

Real-space Chern number

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

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

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

Phys. Rev. B 84, 241106® (2011)

Kernel polynomial for topological invariants in real-space

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

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

With a kernel polynomial tensor network algorithm

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

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

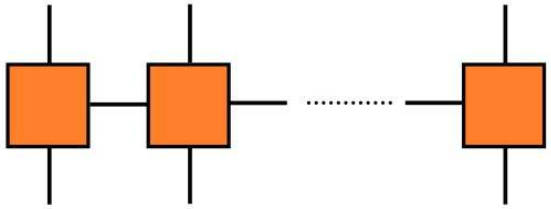
$$T_0 = 1 \text{ and } T_1(x) = x$$

arXiv:2506.05230 (2025)

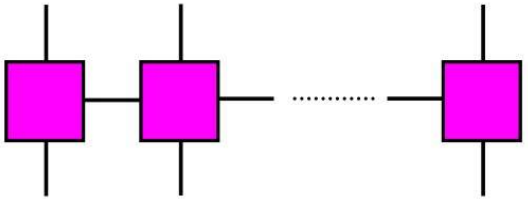
Phys. Rev. B 84, 241106® (2011)

Computing Chern numbers with tensor networks

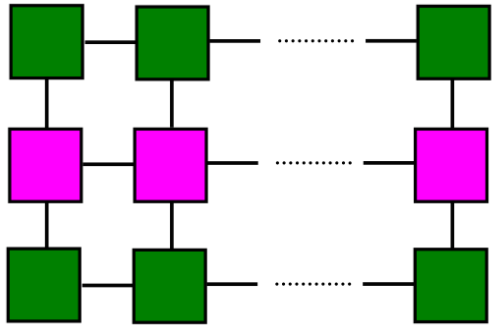
Density matrix as tensor network $\hat{P} = \int_{-\infty}^{\varepsilon_F} \delta(\omega - \hat{H}) d\omega =$



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)

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

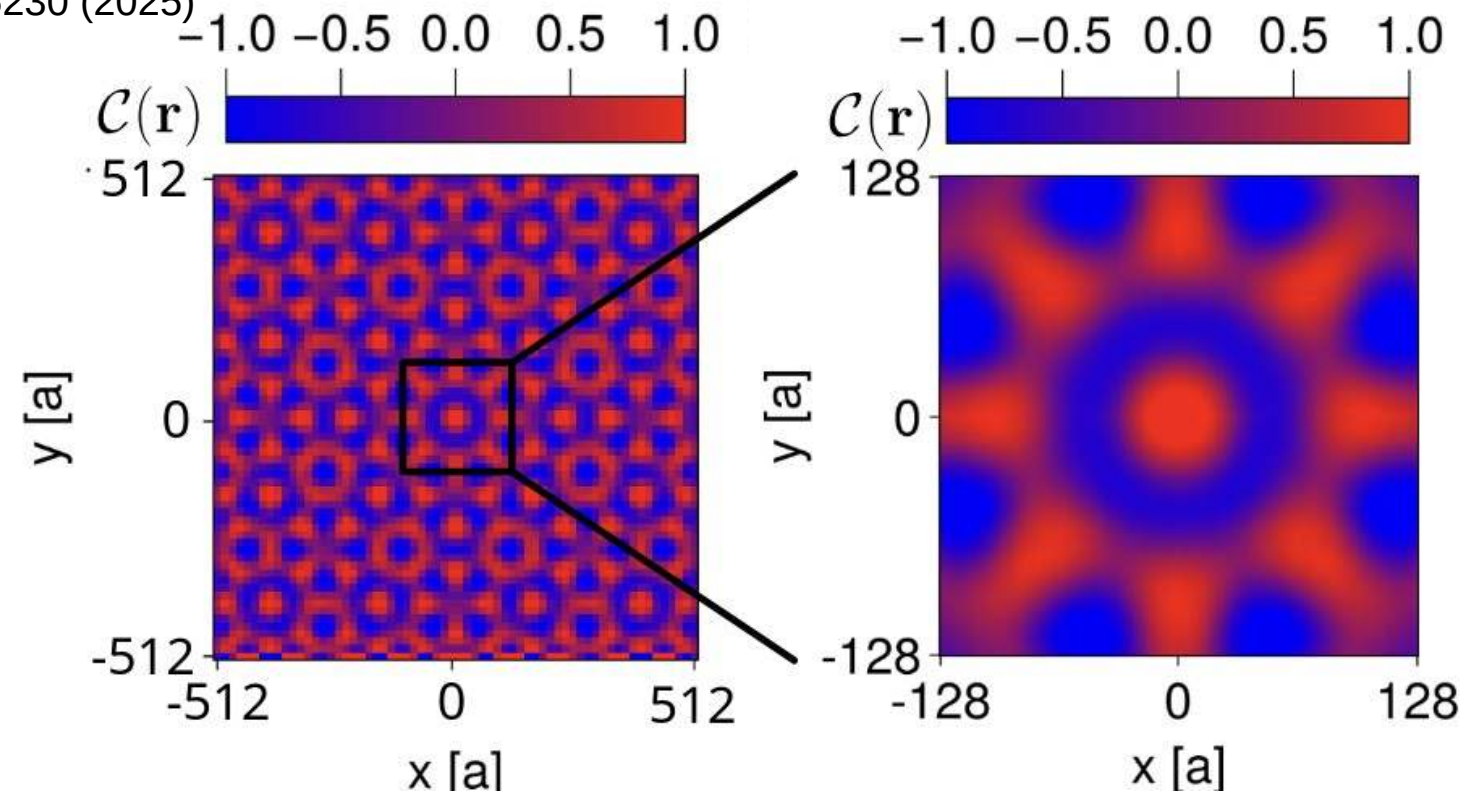
Tensor-network Chern marker

$$\hat{\mathcal{C}}_\alpha = 2\pi i \left(\begin{array}{c} \hat{\mathcal{Q}} \\ \hat{\mathcal{Y}}^\Lambda_\alpha \\ \hat{\mathcal{P}} \\ \hat{\mathcal{X}}^\Lambda_\alpha \\ \hat{\mathcal{Q}} \end{array} \right. - \left. \begin{array}{c} \hat{\mathcal{P}} \\ \hat{\mathcal{Y}}^\Lambda_\alpha \\ \hat{\mathcal{Q}} \\ \hat{\mathcal{X}}^\Lambda_\alpha \\ \hat{\mathcal{P}} \end{array} \right)$$

arXiv:2506.05230 (2025)

Chern mosaic in a 8-fold topological quasicrystal

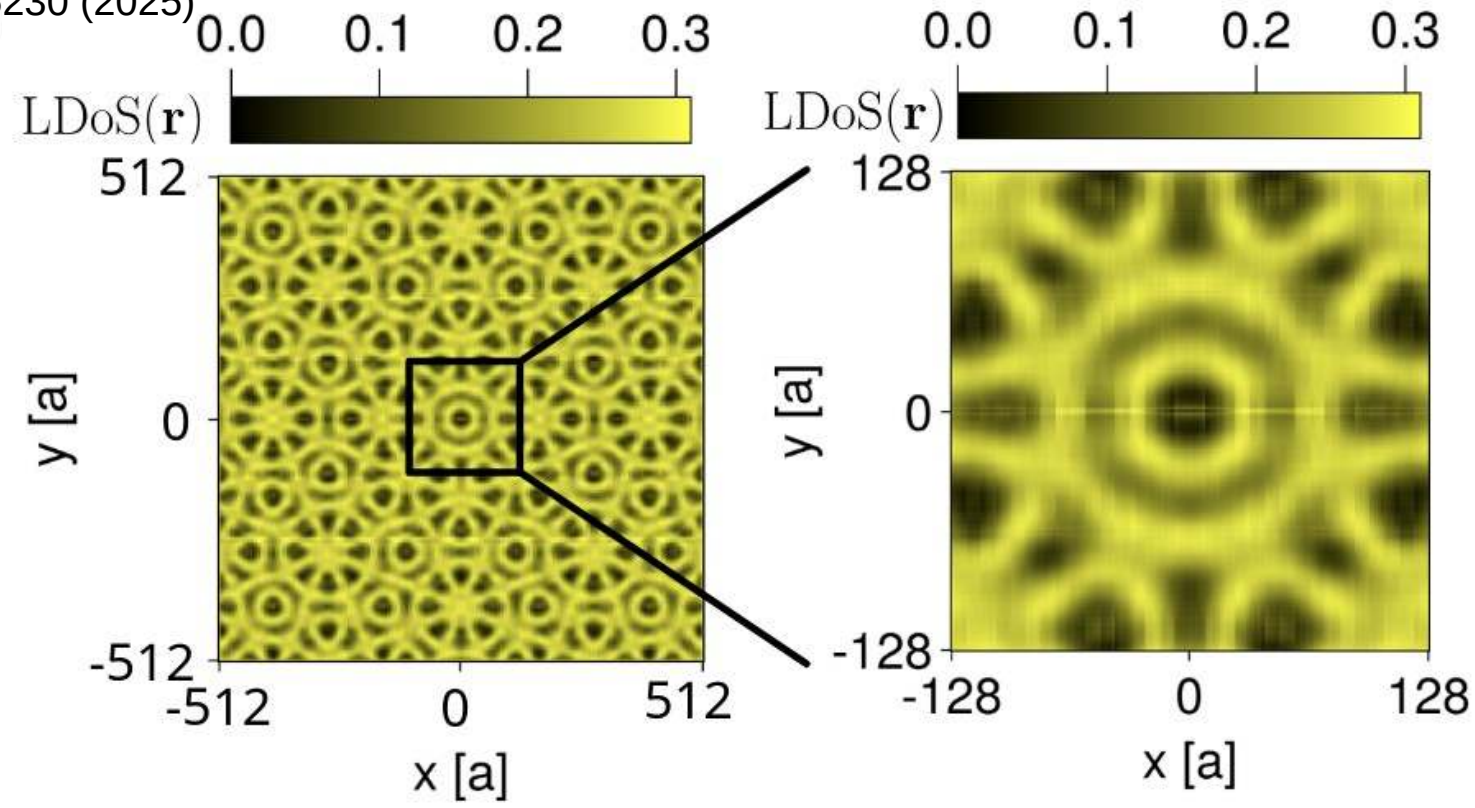
arXiv:2506.05230 (2025)



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

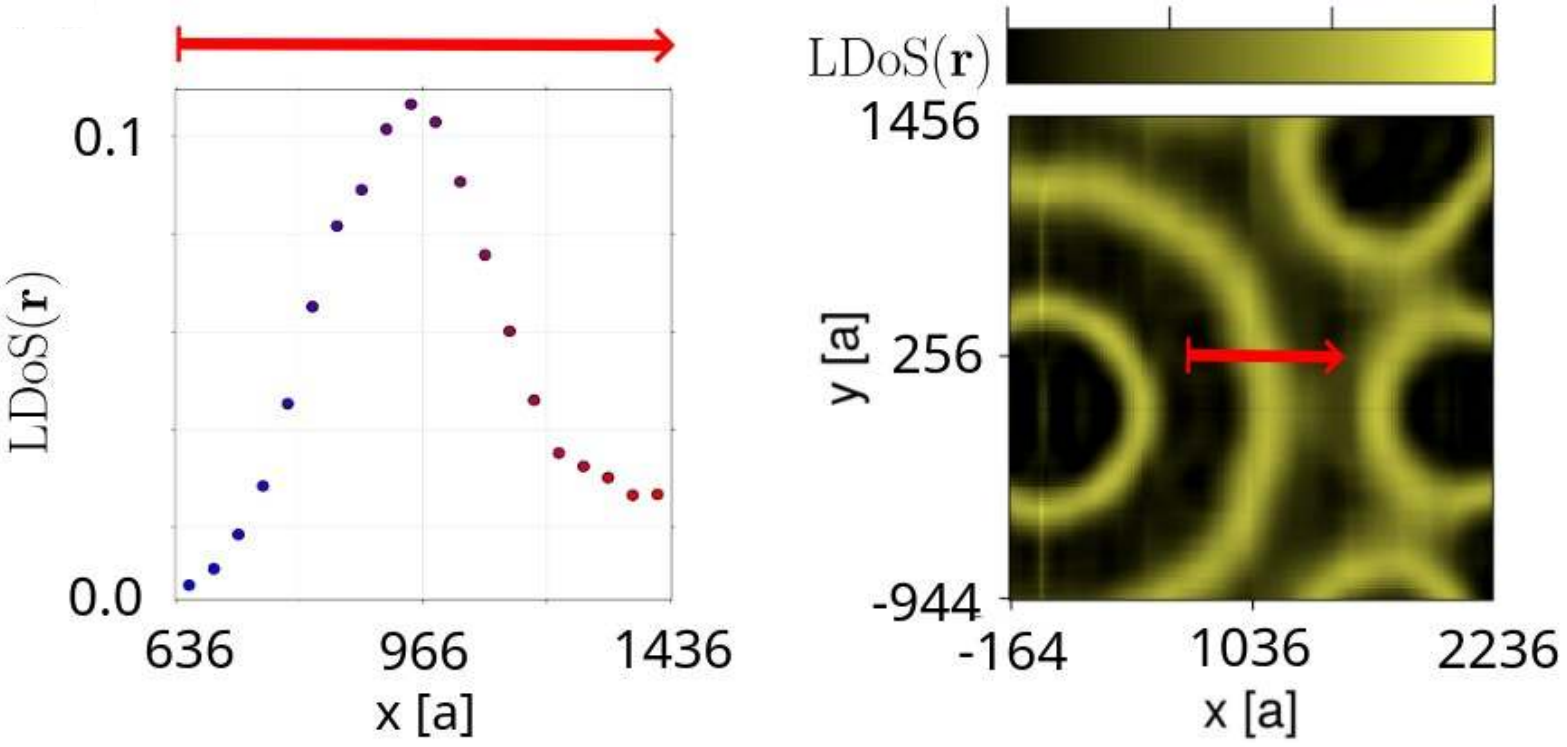
Topological modes in a 8-fold topological quasicrystal

arXiv:2506.05230 (2025)



Topological modes appear between topological domains in real space

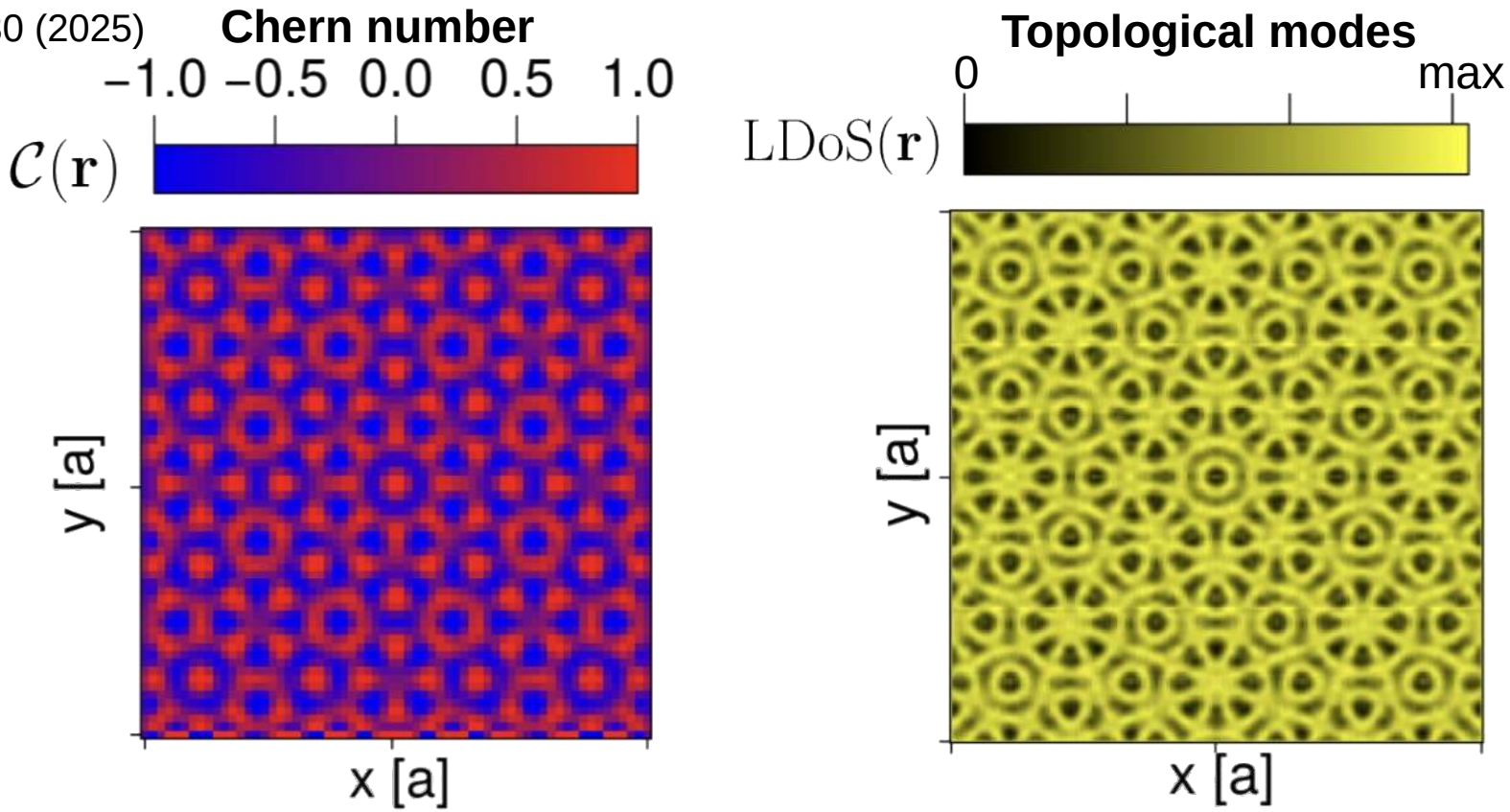
Zero modes across topological quasicrystalline domain



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

Chern mosaic and topological modes in a quasicrystal

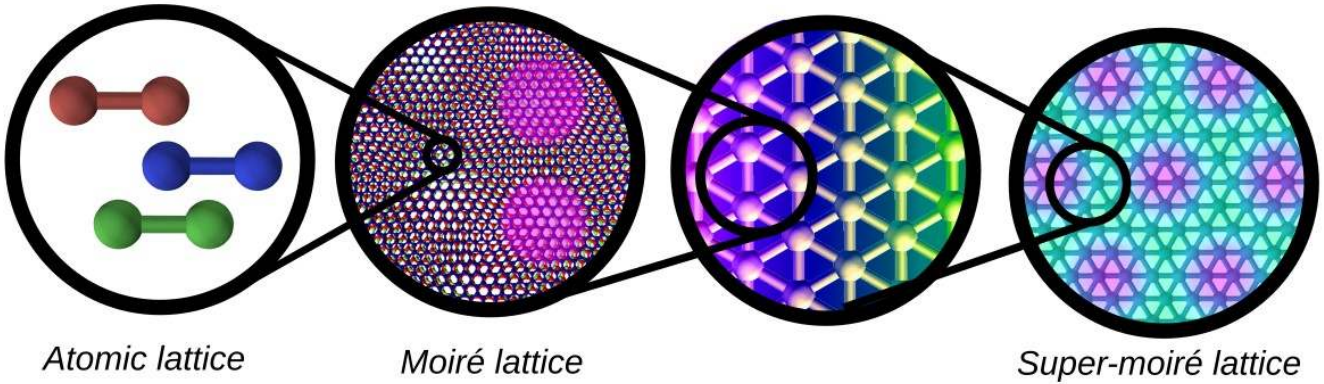
arXiv:2506.05230 (2025)



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

Take home

Exponentially large single-particle problems encoded in a quantum many-body space can be solved by leveraging quantum many-body tensor networks



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Finnish Quantum Flagship FQF

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Institute Q

J&AE JANE AND AATOS ERKKO FOUNDATION

Research Council of Finland

arXiv:2507.04262 (2025) *arXiv:2503.04373 (2025)* *arXiv:2506.05230 (2025)*