Solving interacting super-moire materials with tensor network machine learning

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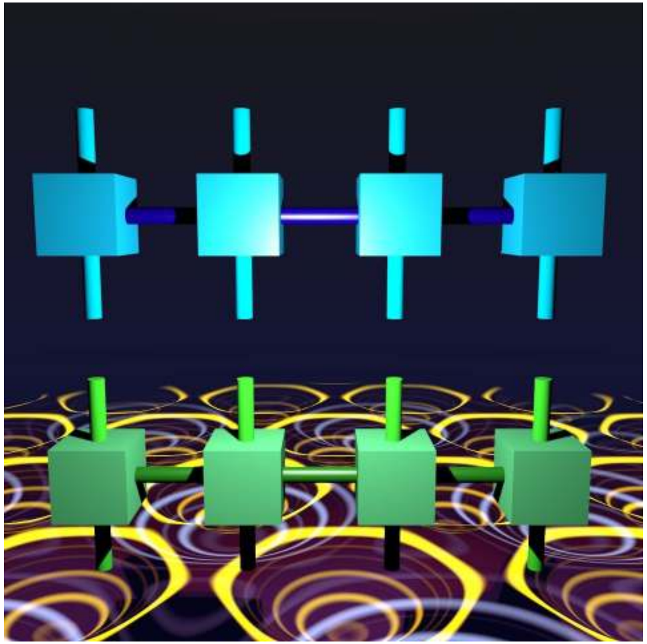
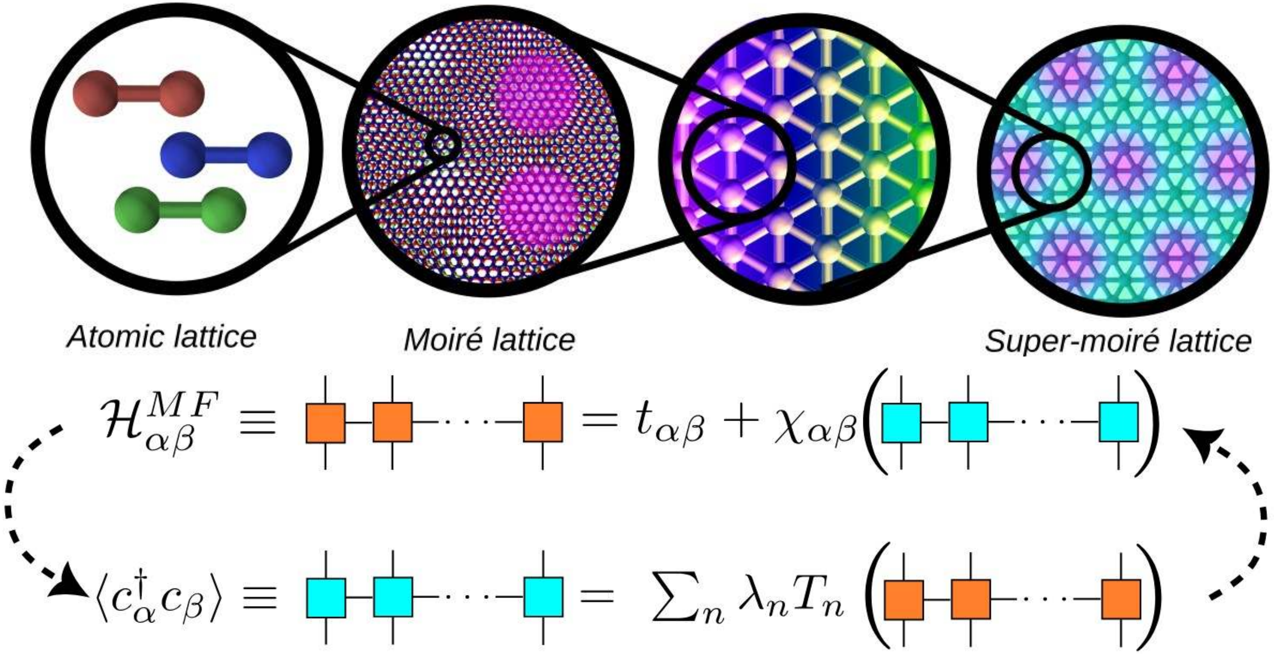
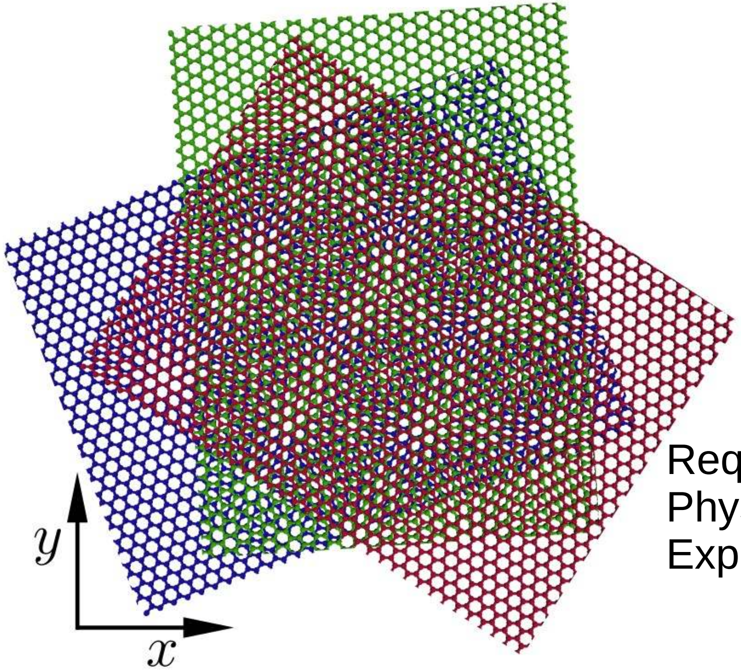


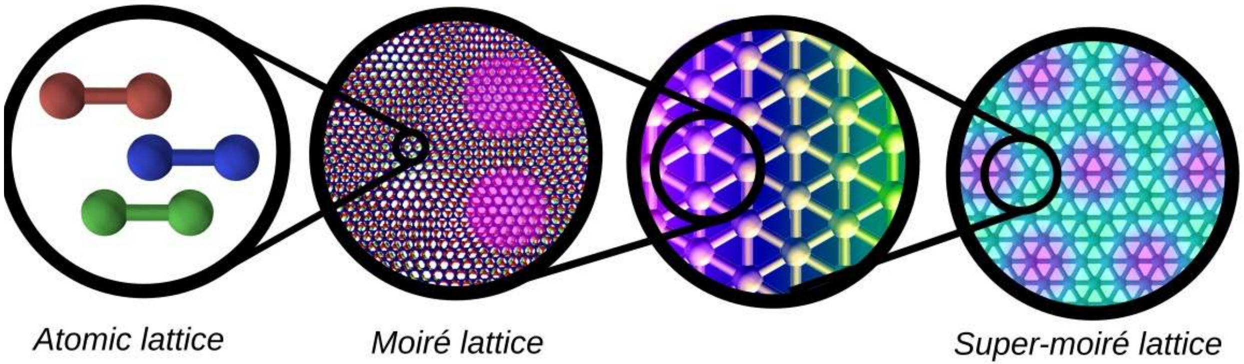


AI 4 Science: from molecules to materials, Aalto University, May 27th 2025

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?

Behind the scenes

Yitao Sun

Tiago Antão

Marcel Niedermeier

Adolfo Fumega

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

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)**

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

The challenge of correlated super-moire materials

Hamiltonian describing electrons in a super-moire material

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

Mean-field treatment of the interacting Hamiltonian

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

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?

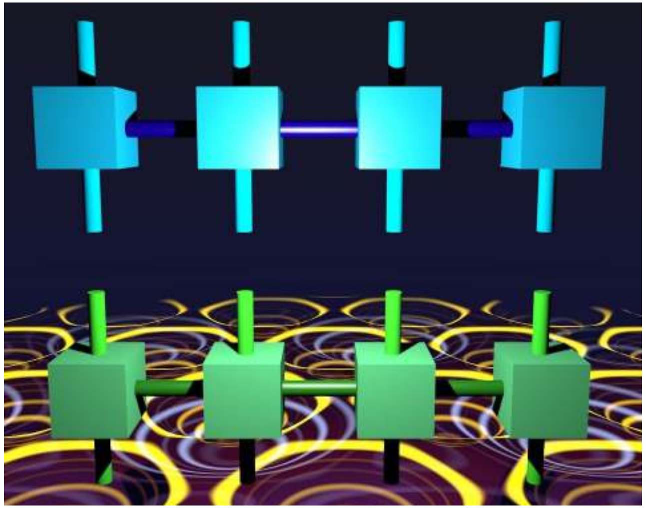
(even before considering the time required to solve it)

Dealing with exponentially large spaces: the quantum many-body problem

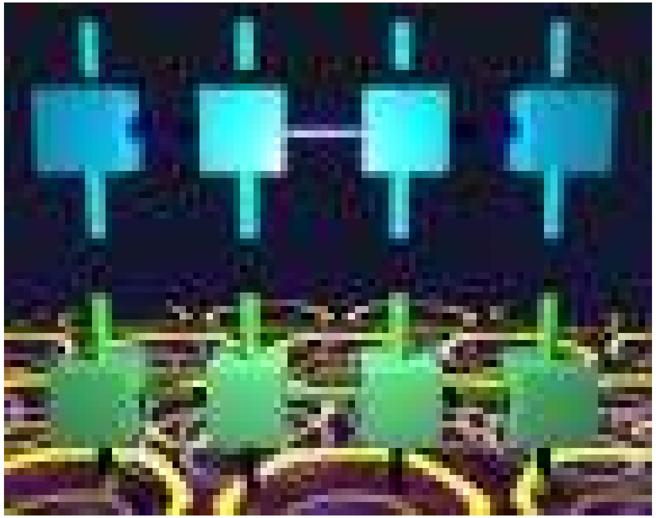
A many-body wavefunction a is a very high dimensional object (2^L coefficients)

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

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



“True wavefunction”



“Tensor-network wavefunction”

Dealing with exponentially large spaces: the quantum many-body problem

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

We need to determine in total 2^L coefficients

Is there an efficient way of storing so many coefficients?

Tensor networks allow parametrizing many-body wavefunctions as

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

$L\chi^2$ parameters

Full wavefunction

Matrix product state

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

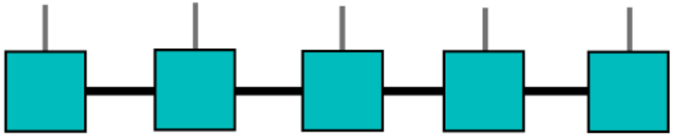
Annals of Physics 326, 96 (2011)

Exponentially large algebra with tensor networks

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

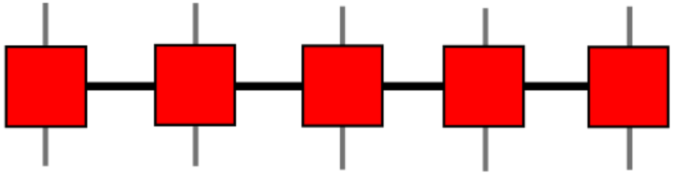
vector

$$|\Psi\rangle \equiv$$

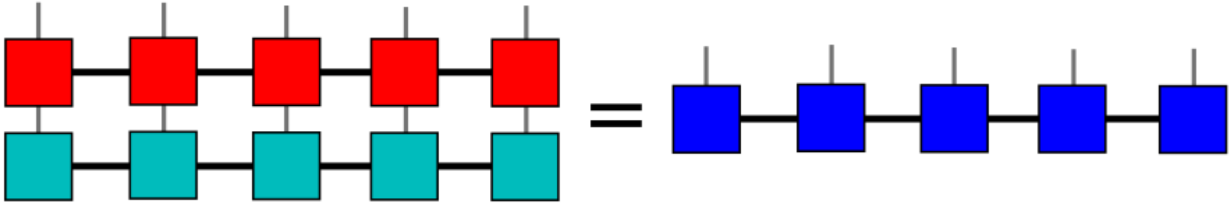


matrix

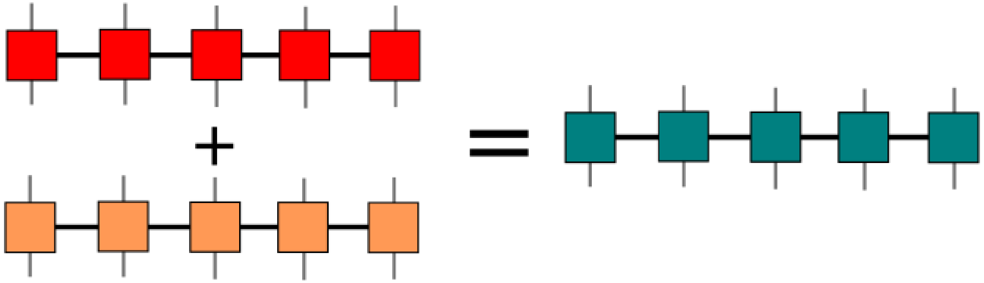
$$\hat{A} \equiv$$



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



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

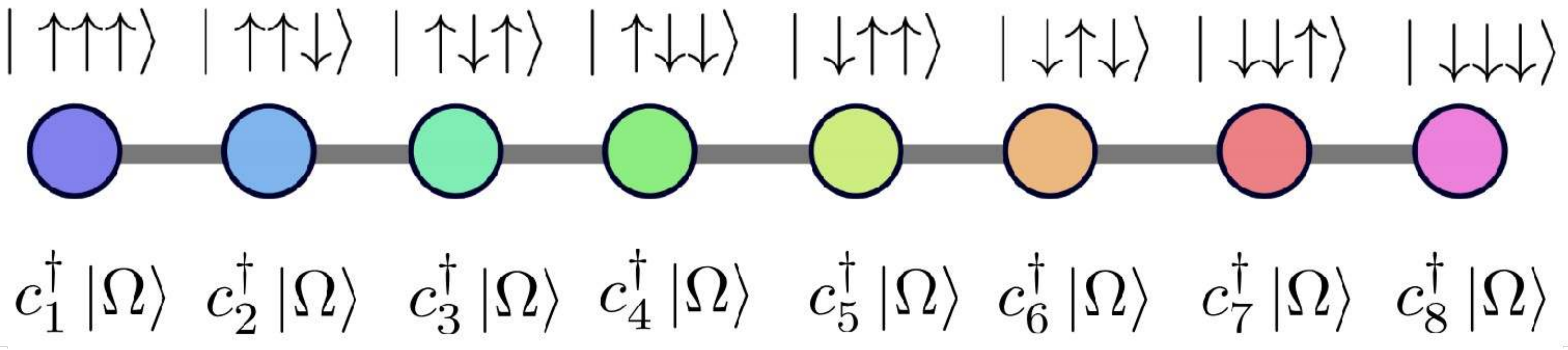


Tensor network machine learning for single particle problems

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

Many-body basis

Single particle basis



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?

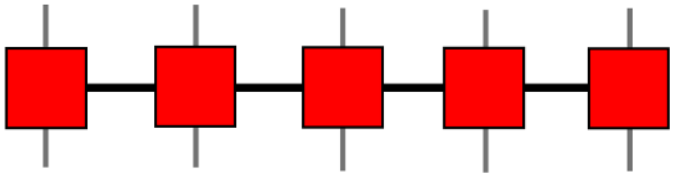
With quantics tensor-cross interpolation: ***<u>a quantum-inspired active learning algorithm</u>***

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

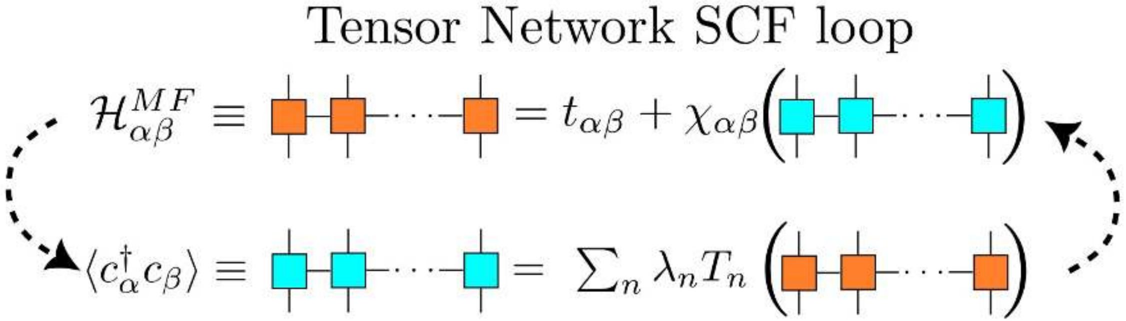
Self-consistent electronic interactions with tensor networks

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

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



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



Kernel polynomial tensor network algorithm

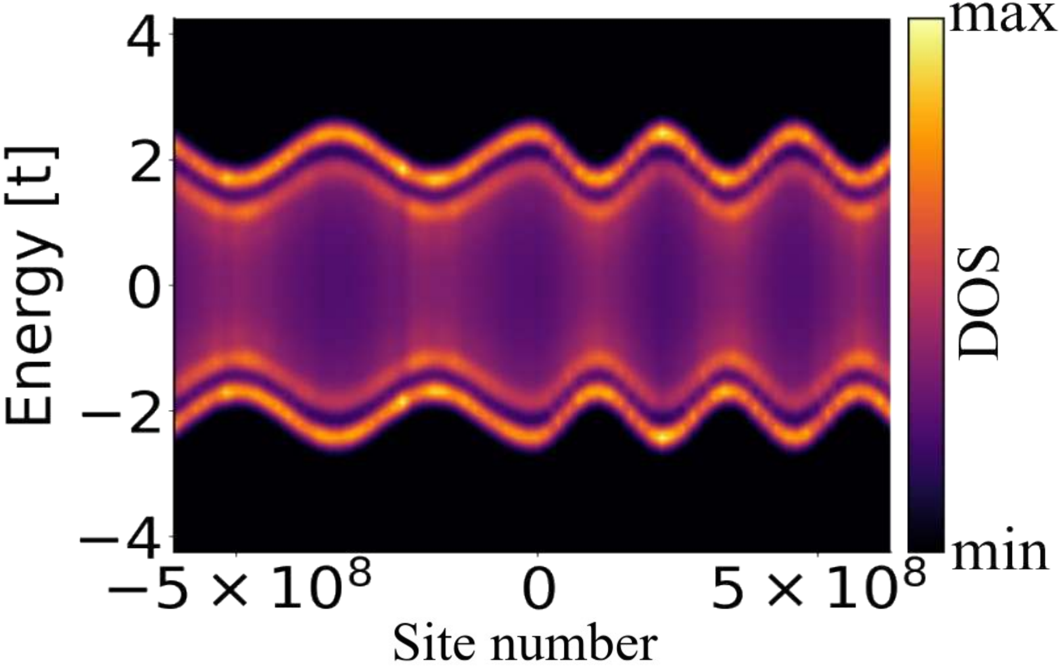
$$\langle c^\dagger_\alpha c_\beta \rangle = \langle \alpha | \Xi(\mathcal{H}^{MF}) | \beta \rangle$$

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

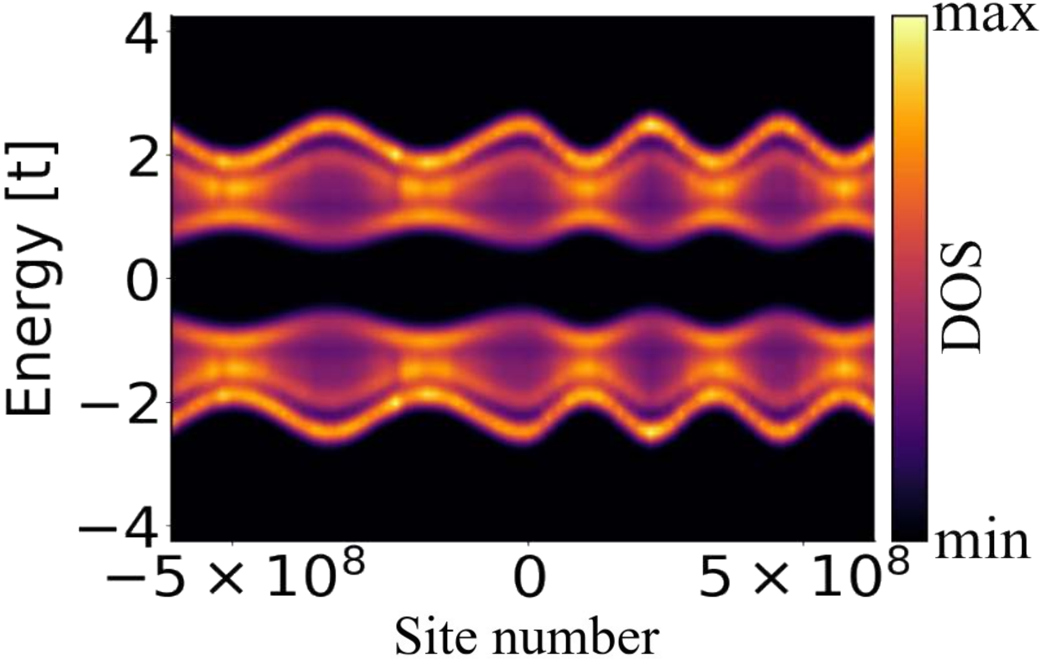
arXiv:2503.04373 (2025)

Solving billion-size super-moire materials

Without interactions



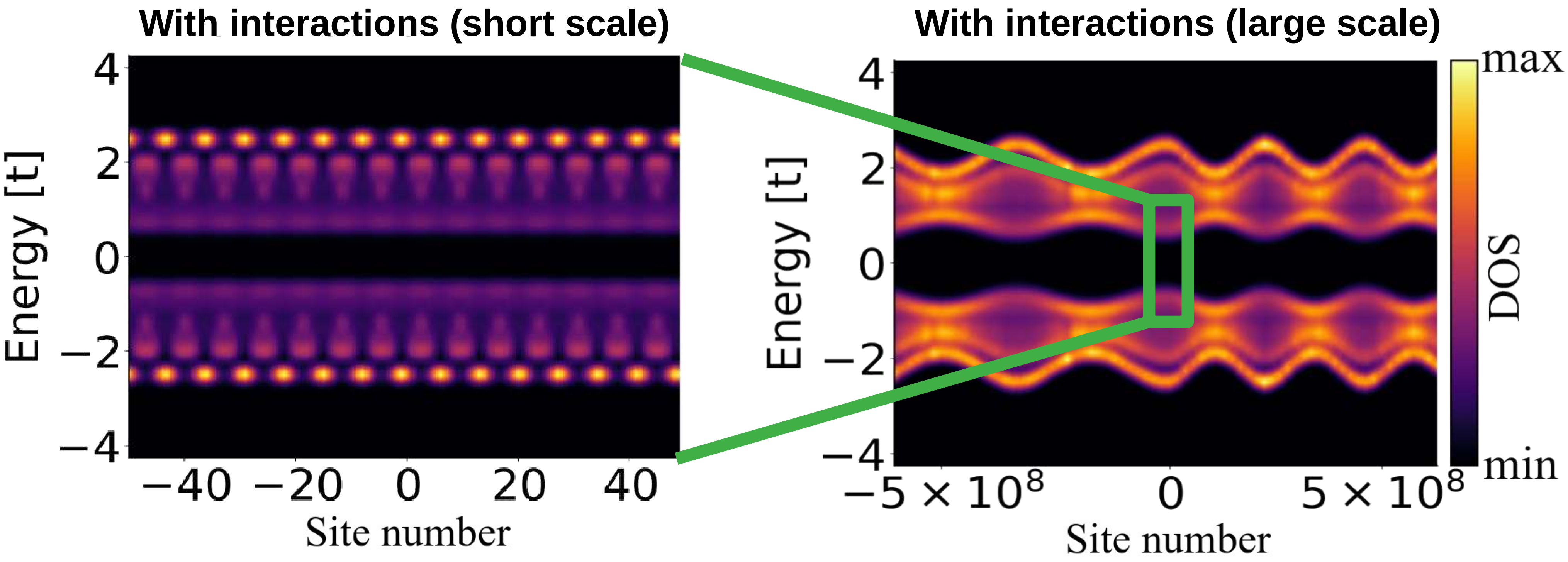
With interactions



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

arXiv:2503.04373 (2025)

Solving billion-size super-moire materials

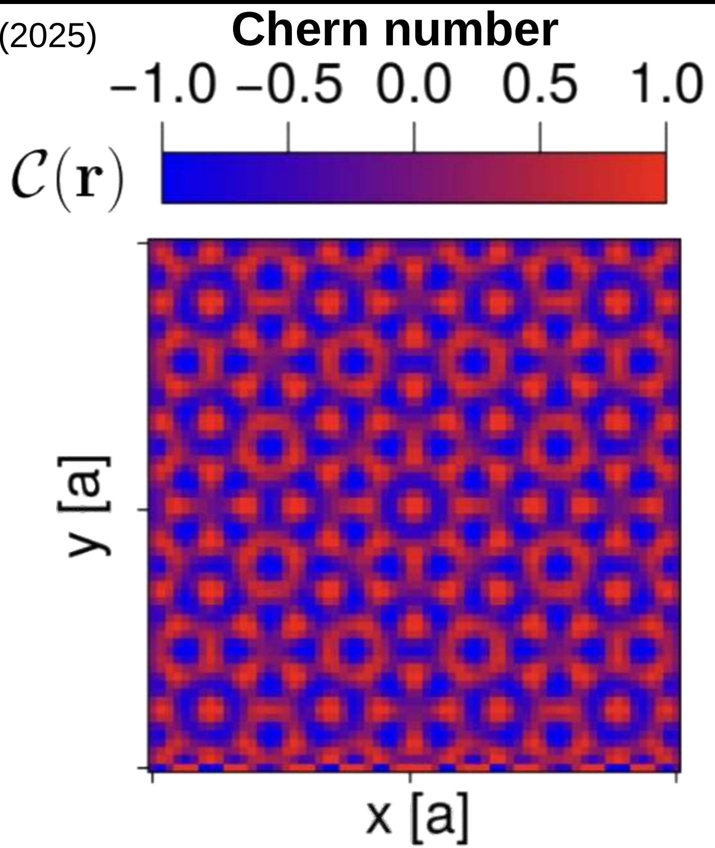


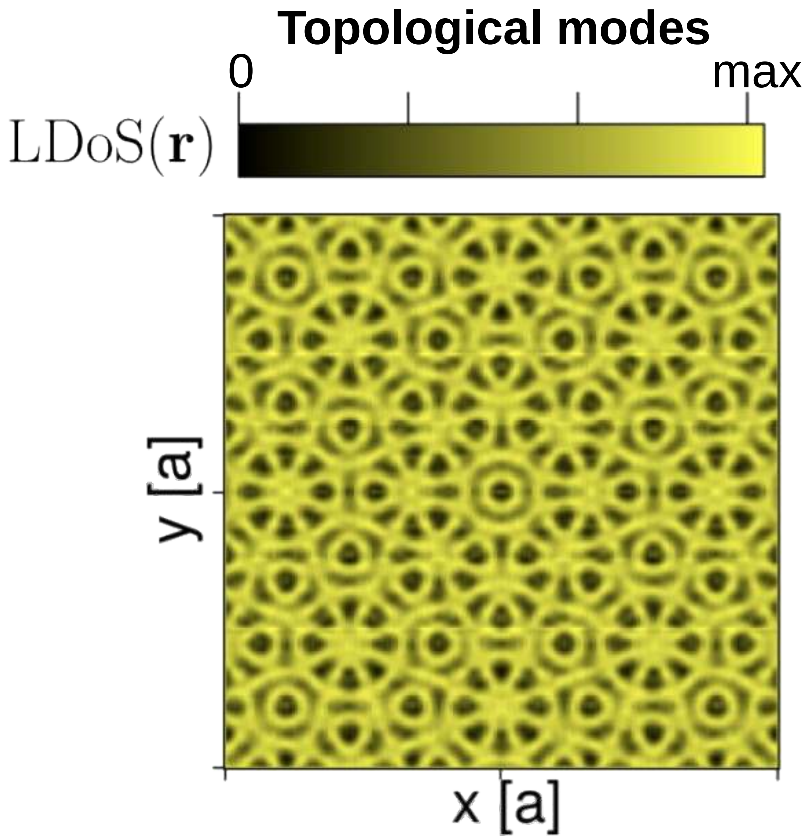
Tensor networks allow to solve selfconsistently a super-moire with one billion sites

arXiv:2503.04373 (2025)

Super-moire topological matter with tensor networks

arXiv:2506.05230 (2025)

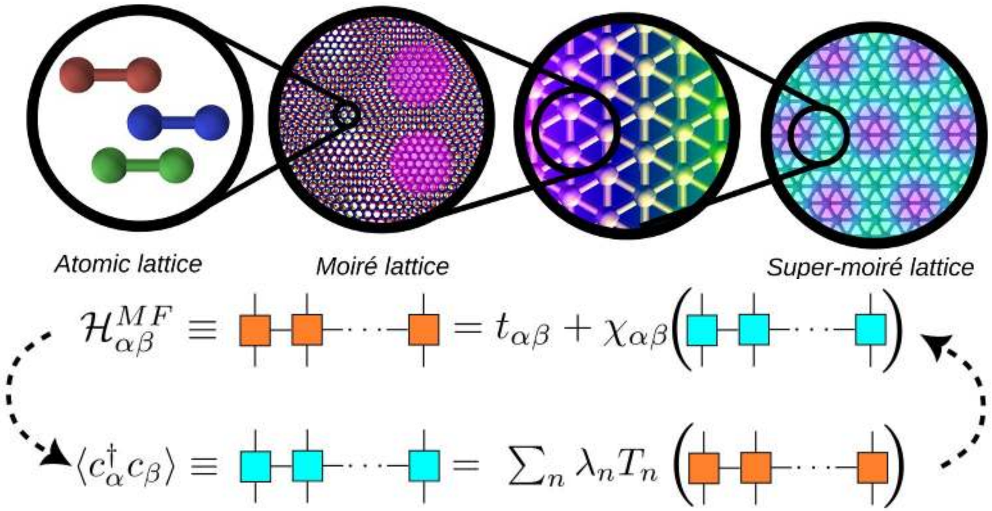




Tensor networks allow computing topology in exceptionally large super-moire systems

Take home

Tensor network machine learning allows solving exponentially large electronic structure problems, reaching the regime required for super-moire materials



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arXiv:2503.04373 (2025)
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