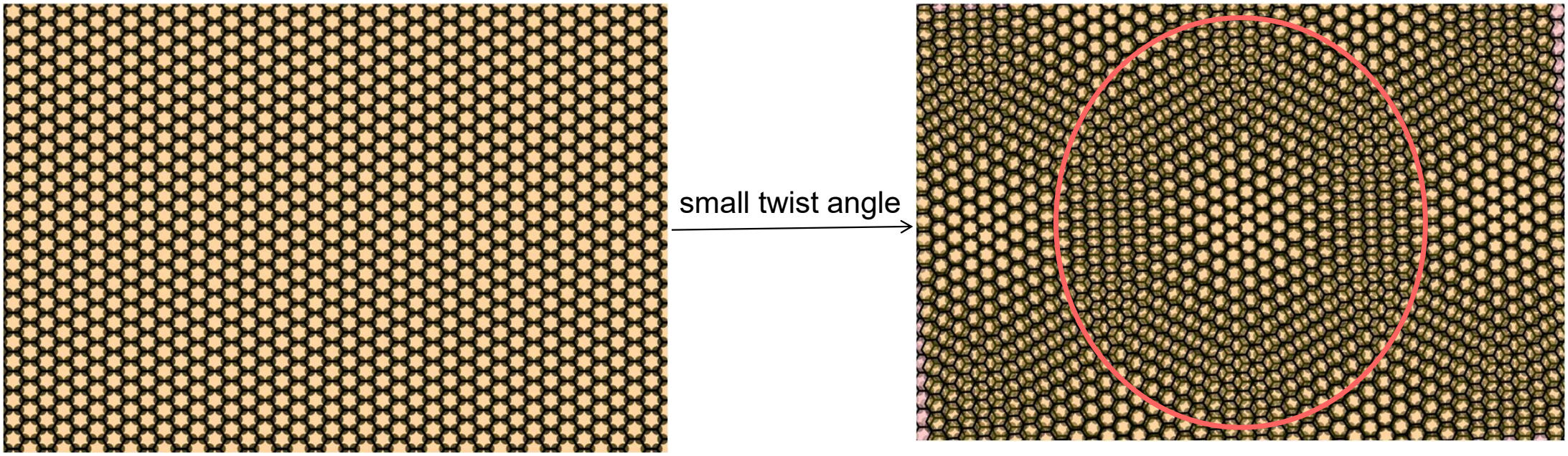
Aalto-yliopisto
Aalto-universitetet
Aalto University

Self-consistent tensor network method for correlated super-moiré matter beyond one billion sites

Yitao Sun
Correlated Quantum Materials group
Aalto University

Contents

Background: what is a moiré material?



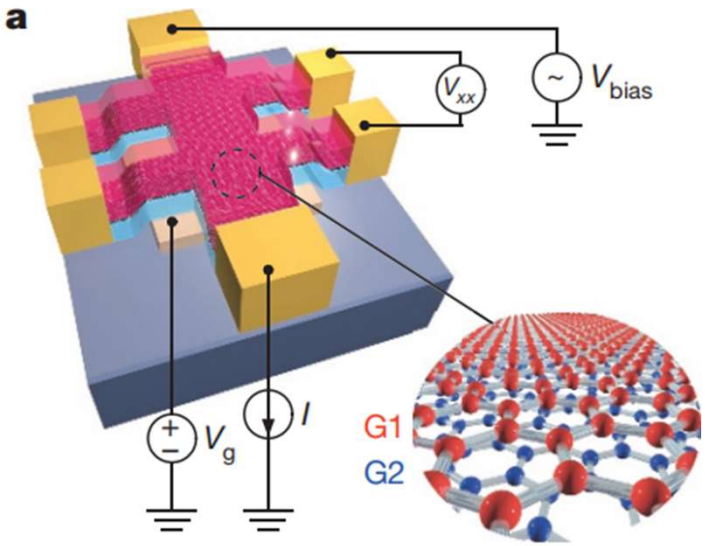
Plain graphene

Twisted angle bilayer graphene

A!

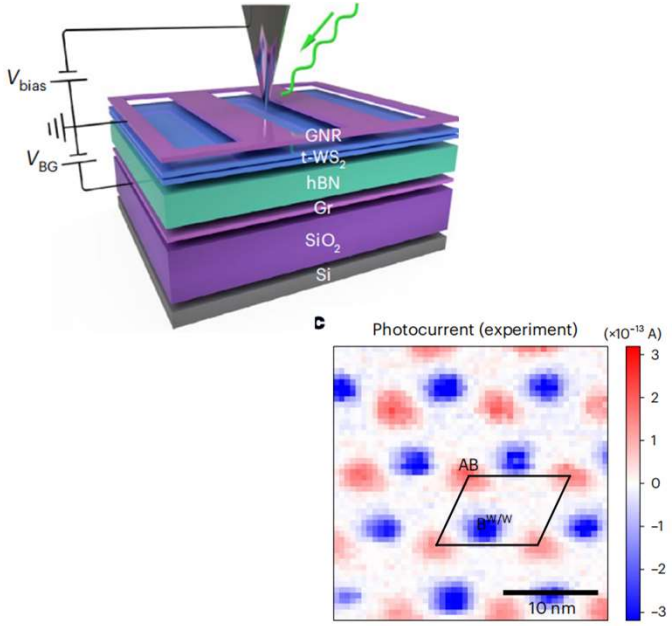
Background: moiré materials in labs

Twisted angle bilayer graphene:



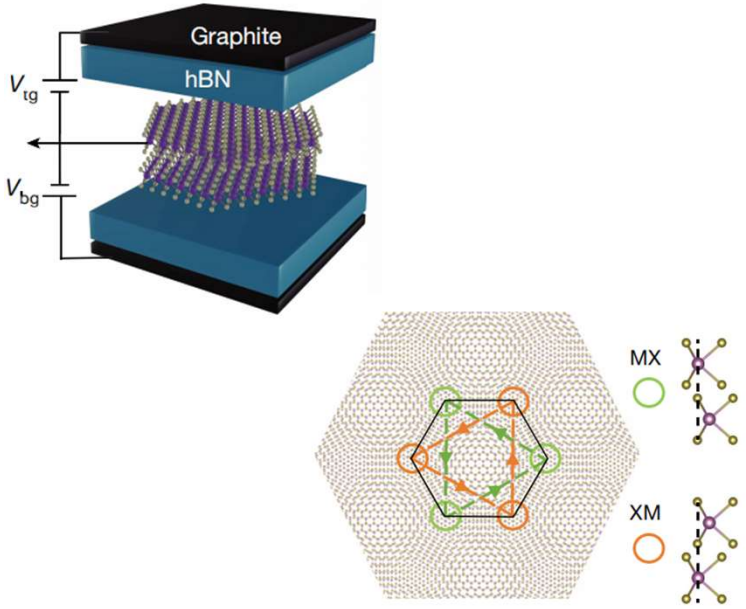
unconventional superconductivity

Twisted angle bilayer WS_2:



moiré exciton

Twisted angle bilayer $MoTe_2$:



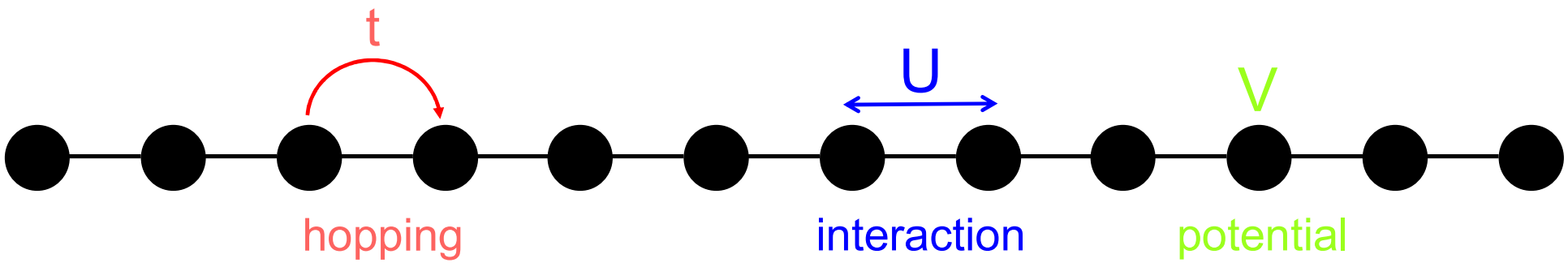
fractional Chern insulator

A!

Cao Y, Fatemi V, Fang S, et al. Unconventional superconductivity in magic-angle graphene superlattices[J]. Nature, 2018, 556(7699): 43-50.
Li H, Xiang Z, Naik M H, et al. Imaging moiré excited states with photocurrent tunnelling microscopy[J]. Nature materials, 2024, 23(5): 633-638.
Cai J, Anderson E, Wang C, et al. Signatures of fractional quantum anomalous Hall states in twisted MoTe2[J]. Nature, 2023, 622(7981): 63-68.

Background: tight-binding Hamiltonian

For a 1D fermionic system:



Tight-binding Hamiltonian:

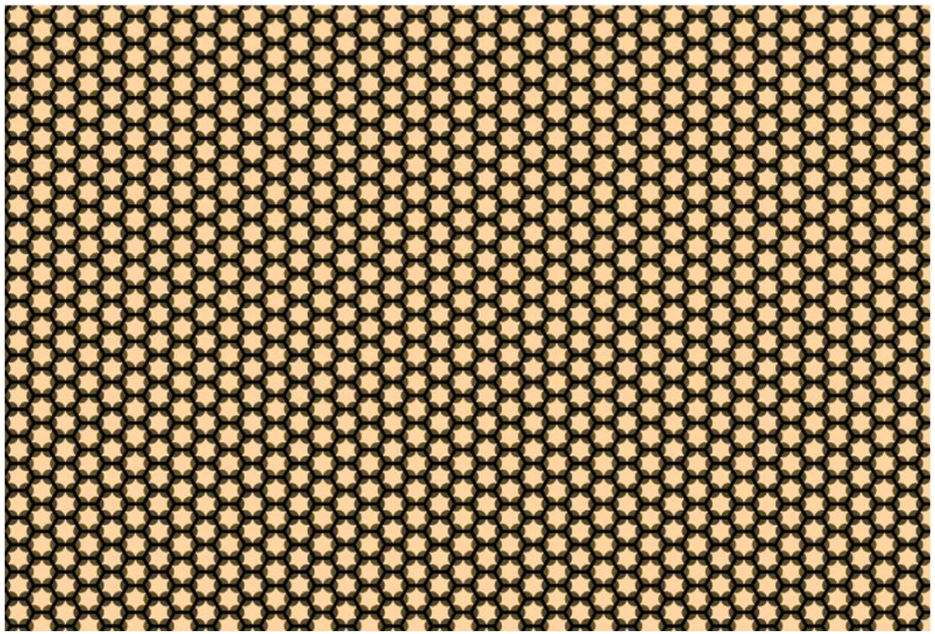
$$H = \sum_{i,j} t(c_i c_j^\dagger + h.c.) + \sum_i V n_i + \sum_{i,j} U n_i n_j$$

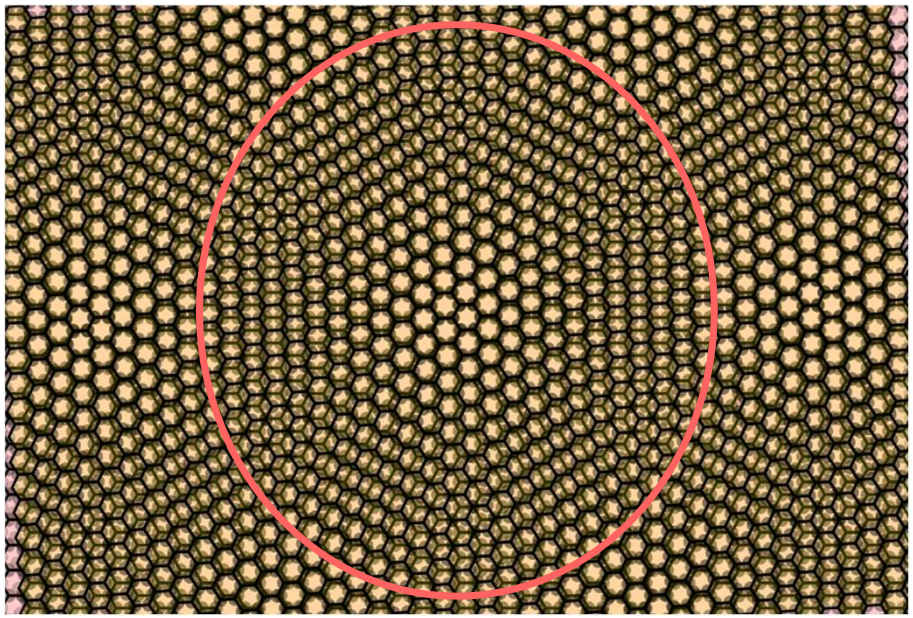
$$n_i = c_i^\dagger c_i$$

A matrix depending on the size of unit cell

A!

Background: size of a unit cell for moiré



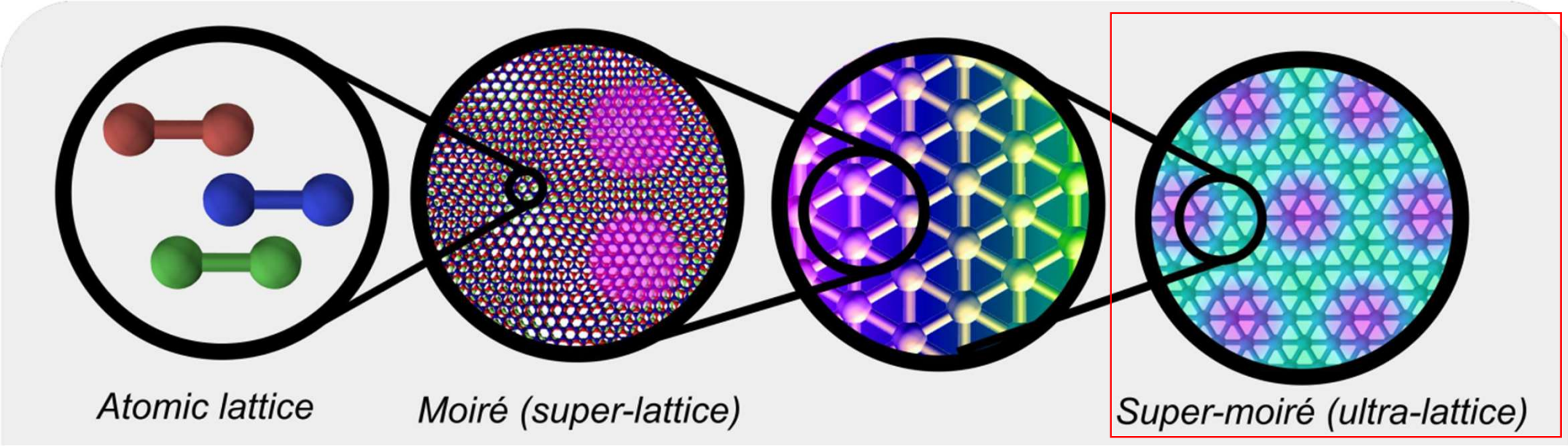


Plain graphene
2 atoms in a unit cell

Twisted angle bilayer graphene
>10000 atoms in a moiré unit cell

A!

Motivation: super-moiré materials



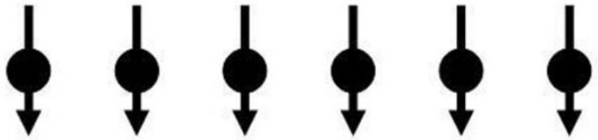
2 or even more
moiré coexist

>$(10000)^2$ atoms
in a unit cell

Hamiltonian with size of $10^8 \times 10^8$!

A!

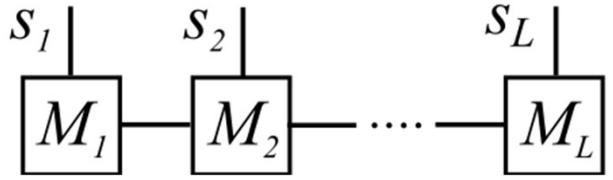
The idea of tensor network



An L-site spin-1/2 chain

The state:

$$\begin{bmatrix} 0 \\ 0 \\ 0 \\ \\ 0 \\ \\ \vdots \\ 0 \end{bmatrix} \quad 2^L$$

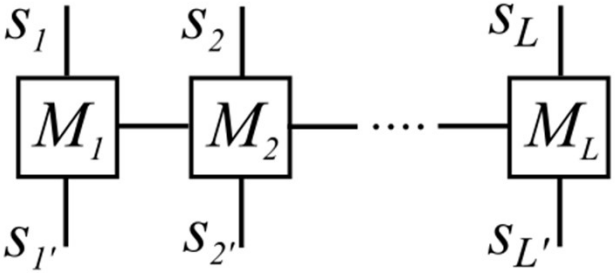


Matrix Product State (MPS)

The Hamiltonian:

$$\begin{bmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 1 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \ddots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & 1 \\ 0 & 0 & 0 & 0 & \cdots & 0 \end{bmatrix} \quad 2^L$$

2^L



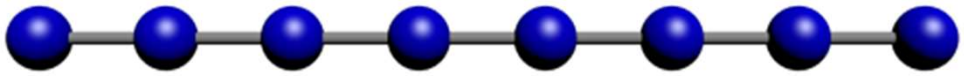
Matrix Product Operator (MPO)

with bond dimension χ

A!

A tensor network representation for tight-binding system

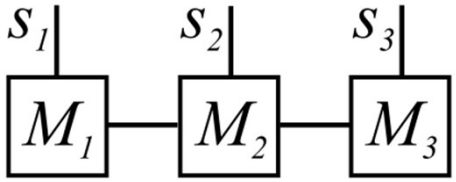
normal tight-binding basis:



8-site spinless fermionic chain

pseudo-spin (quantics) basis: $|\uparrow\uparrow\uparrow\rangle$ $|\uparrow\uparrow\downarrow\rangle$ $|\uparrow\downarrow\uparrow\rangle$ $|\uparrow\downarrow\downarrow\rangle$ $|\downarrow\uparrow\uparrow\rangle$ $|\downarrow\uparrow\downarrow\rangle$ $|\downarrow\downarrow\uparrow\rangle$ $|\downarrow\downarrow\downarrow\rangle$

L-site MPS:



A!

Can we achieve this compression?

Aalto-yliopisto
Aalto-universitetet
Aalto University

The general formalism of tensorizing tight-binding system

The trivial single electron Hamiltonian

1D nearest-neighbor (NN) hopping with fermionic basis:

$$\sum_i (c_i c_{i+1}^\dagger + h.c.)$$

2^L

$$\begin{bmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 1 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \ddots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & 1 \\ 0 & 0 & 0 & 0 & \cdots & 0 \end{bmatrix}$$

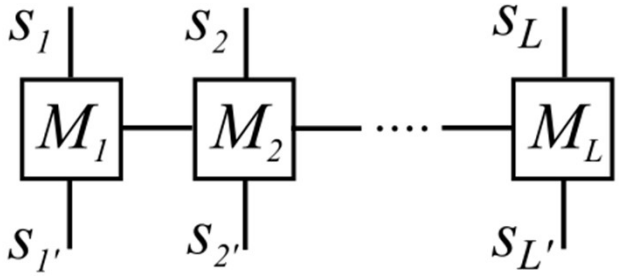
2^L

equivalent

1D NN hopping with pseudo-spin basis:

$$\sum_i (\sigma_l^+ \otimes_{m>l} \sigma_m^- + h.c.)$$

$$\sigma^\pm = \tfrac{1}{2}(\sigma_x \pm i\sigma_y)$$



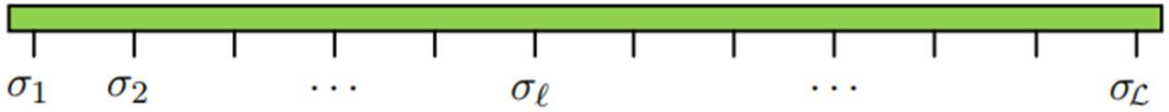
A!

But what if it is non-trivial?

Quantics tensor cross interpolation (QTCI) algorithm

Assume one has a function f(x) with 2^L x:

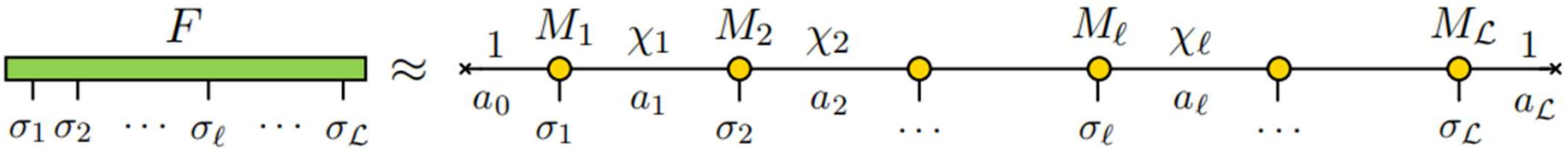
$$F_{\boldsymbol{\sigma}} = f\big(\mathbf{x}(\boldsymbol{\sigma})\big) =$$



binary expression of x

Quantics representation

Tensor cross interpolation:



original function

matrix product state approximation

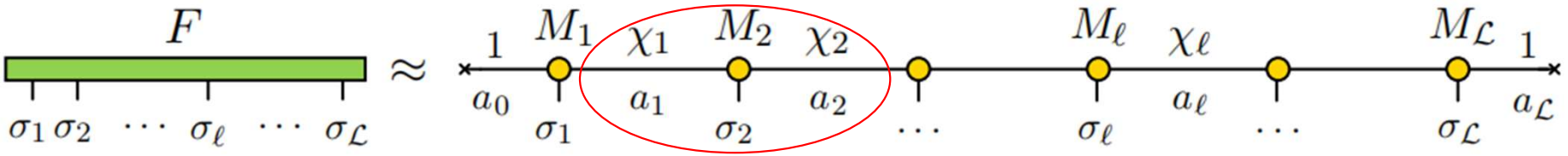
$$F_{\boldsymbol{\sigma}} \approx \widetilde{F}_{\boldsymbol{\sigma}} = \prod_{\ell=1}^{\mathcal{L}} M_\ell^{\sigma_\ell} = [M_1]^{\sigma_1}_{1a_1}[M_2]^{\sigma_2}_{a_1a_2}\cdots[M_{\mathcal{L}}]^{\sigma_{\mathcal{L}}}_{a_{\mathcal{L}-1}1}$$

The QTCI algorithm

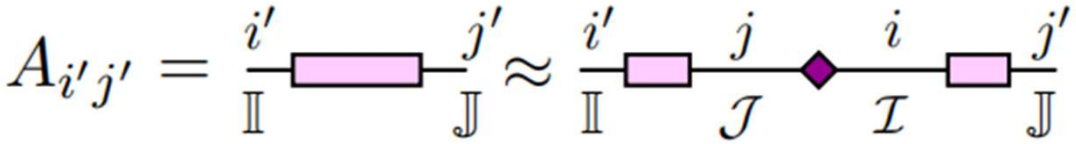
A!

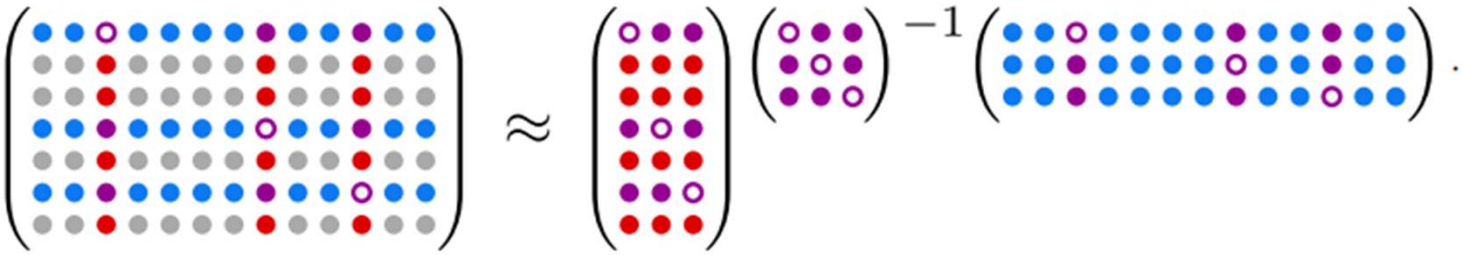
Núñez Fernández Y, Ritter M K, Jeannin M, et al. Learning tensor networks with tensor cross interpolation: new algorithms and libraries[J]. SciPost Physics, 2025, 18(3): 104.

Why we use it?



matrix cross interpolation





approximation of the
whole matrix

only explicitly evaluate
few values

A!

Núñez Fernández Y, Ritter M K, Jeannin M, et al. Learning tensor networks with tensor cross interpolation: new algorithms and libraries[J]. SciPost Physics, 2025, 18(3): 104.

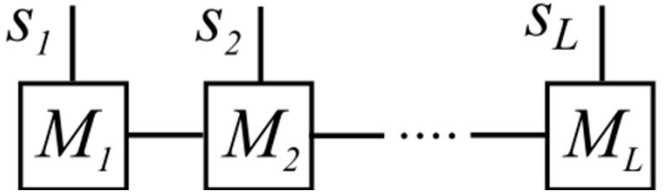
Spatially varying NN term as tensor network

$$\sum_i t(x_i)(c_i c_{i+1}^\dagger + h.c.) \longrightarrow \begin{bmatrix} 0 & t(x_1) & 0 & 0 & \cdots & 0 \\ 0 & 0 & t(x_2) & 0 & \cdots & 0 \\ 0 & 0 & 0 & t(x_3) & \cdots & 0 \\ 0 & 0 & 0 & 0 & \ddots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & t(x_{2^L-1}) \\ 0 & 0 & 0 & 0 & \cdots & 0 \end{bmatrix}$$

now amplitude as function of x

Step 1: Acquire the MPS form of $t(x_i)$:

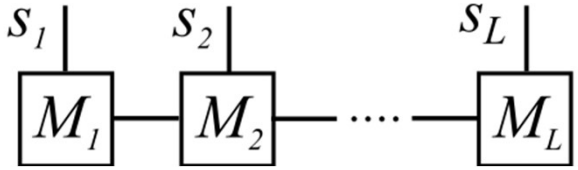
$t(x_i)$ —QTCI→



A!

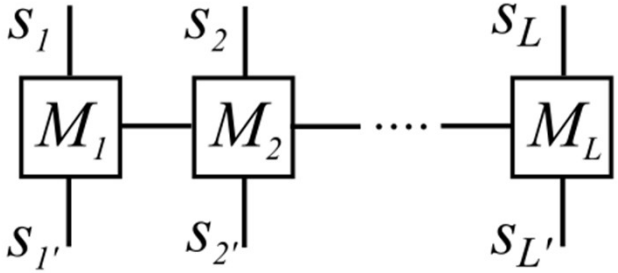
Spatially varying NN term as tensor network

Step 2: Get the diagonal MPO based on the MPS



Adding extra indices

force $s_i = s_{i'}$



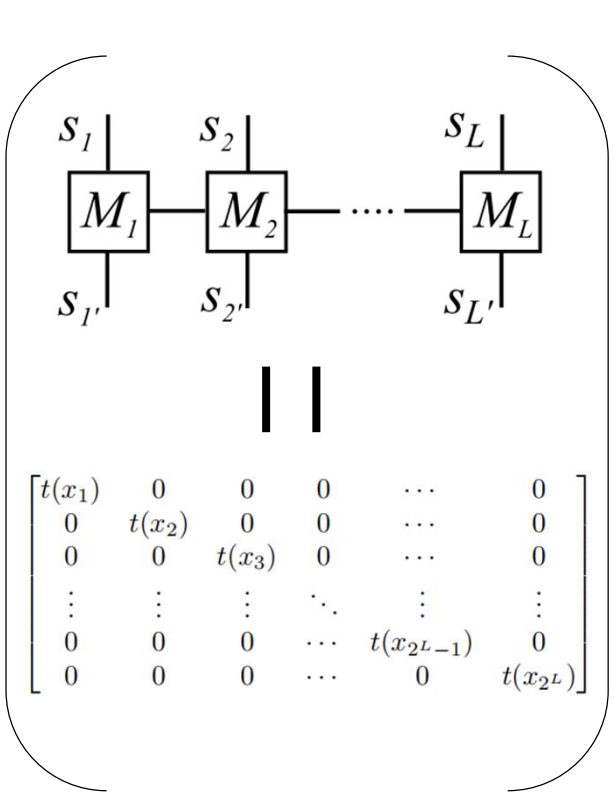
$$\begin{bmatrix} t(x_1) \\ t(x_2) \\ t(x_3) \\ \vdots \\ t(x_{2^L}) \end{bmatrix}$$

$$\begin{bmatrix} t(x_1) & 0 & 0 & 0 & \cdots & 0 \\ 0 & t(x_2) & 0 & 0 & \cdots & 0 \\ 0 & 0 & t(x_3) & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & t(x_{2^L-1}) & 0 \\ 0 & 0 & 0 & \cdots & 0 & t(x_{2^L}) \end{bmatrix}$$

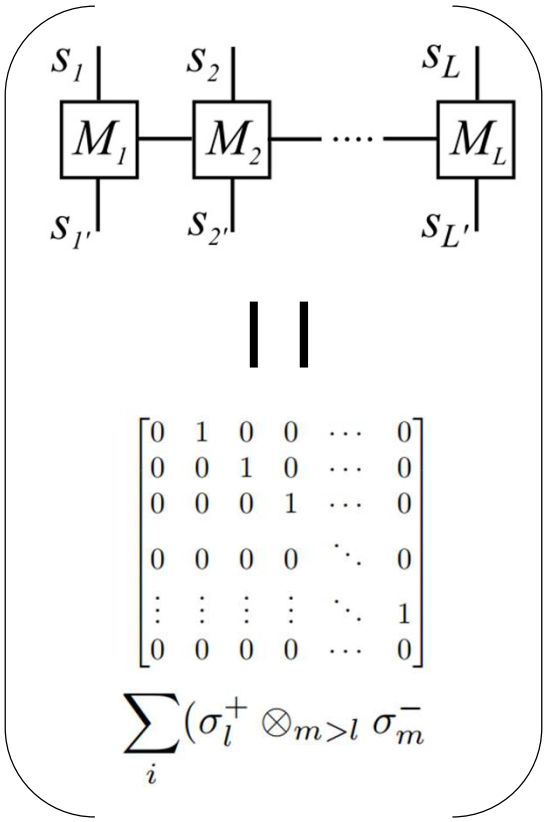
A!

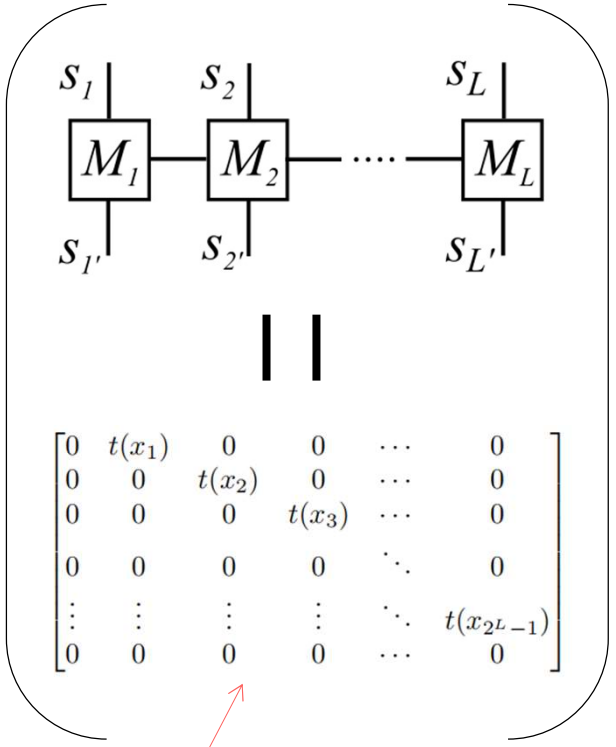
Spatially varying NN term as tensor network

Step 3: Cast the values to the proper position



*





equivalent

$$\sum_i t(x_i)(c_i c_{i+1}^\dagger$$

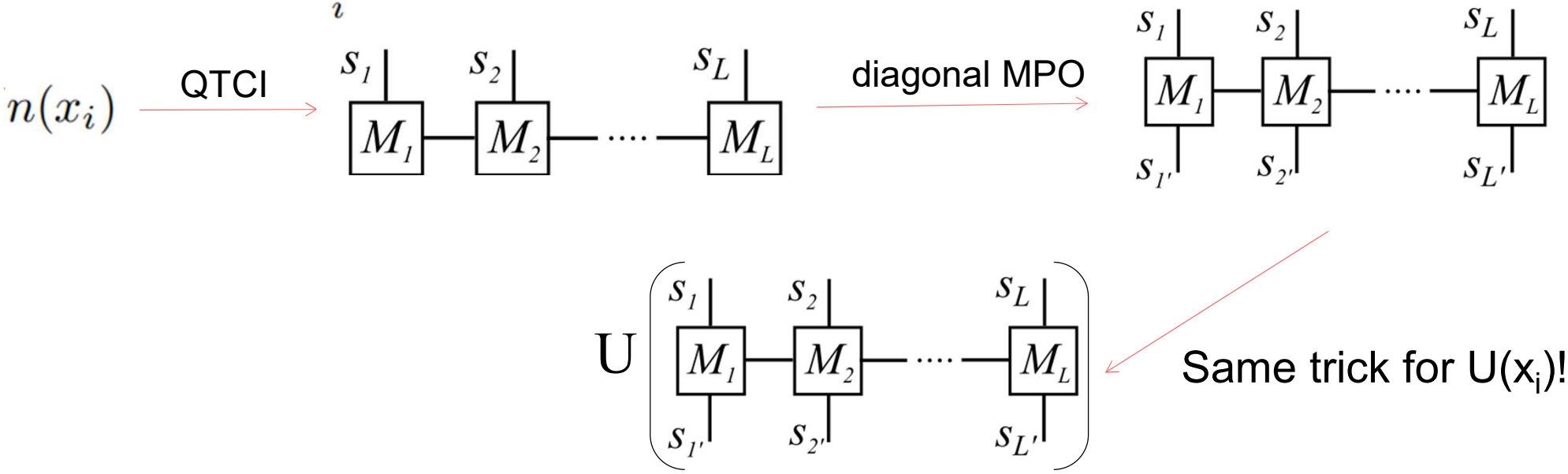
A!

Spatially varying on-site potential

A spatially varying potential term:

$$\sum_i U n(x_i)$$

$n(x_i)$ being the particle density

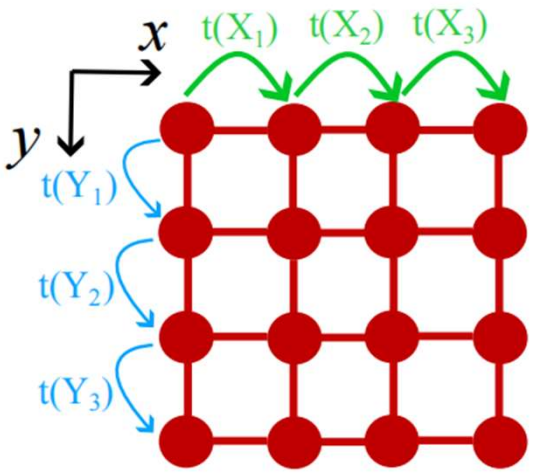


MPO for the on-site potential

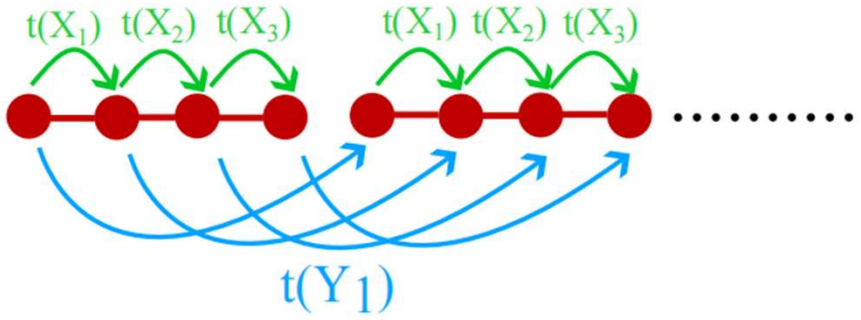
A!

2D tight-binding systems

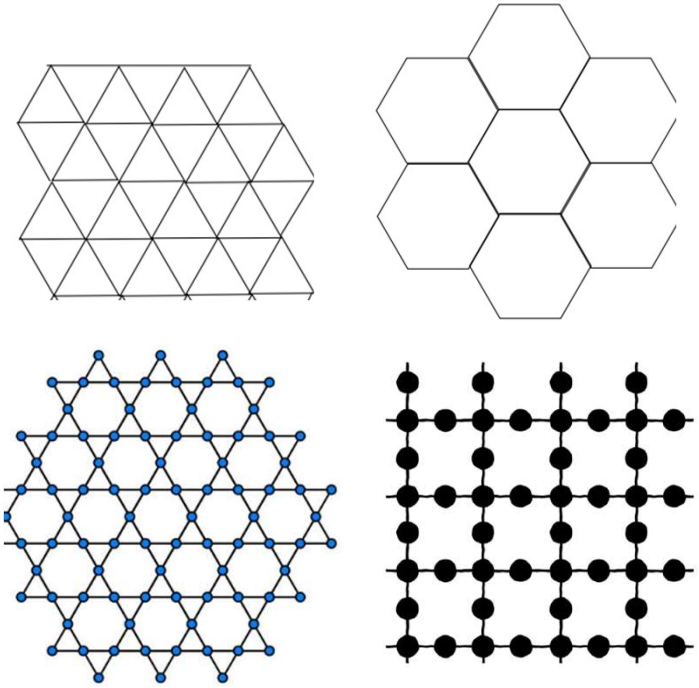
Folding of 2D systems:



as 1D chain:

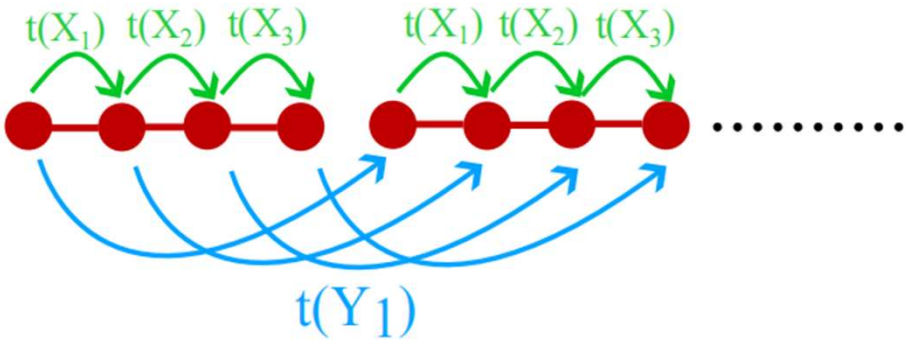


Same trick for:



A!

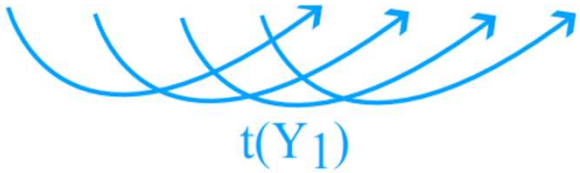
Intra- and inter-chain hoppings



1. Intra-chain hopping:

NN hopping with breaks

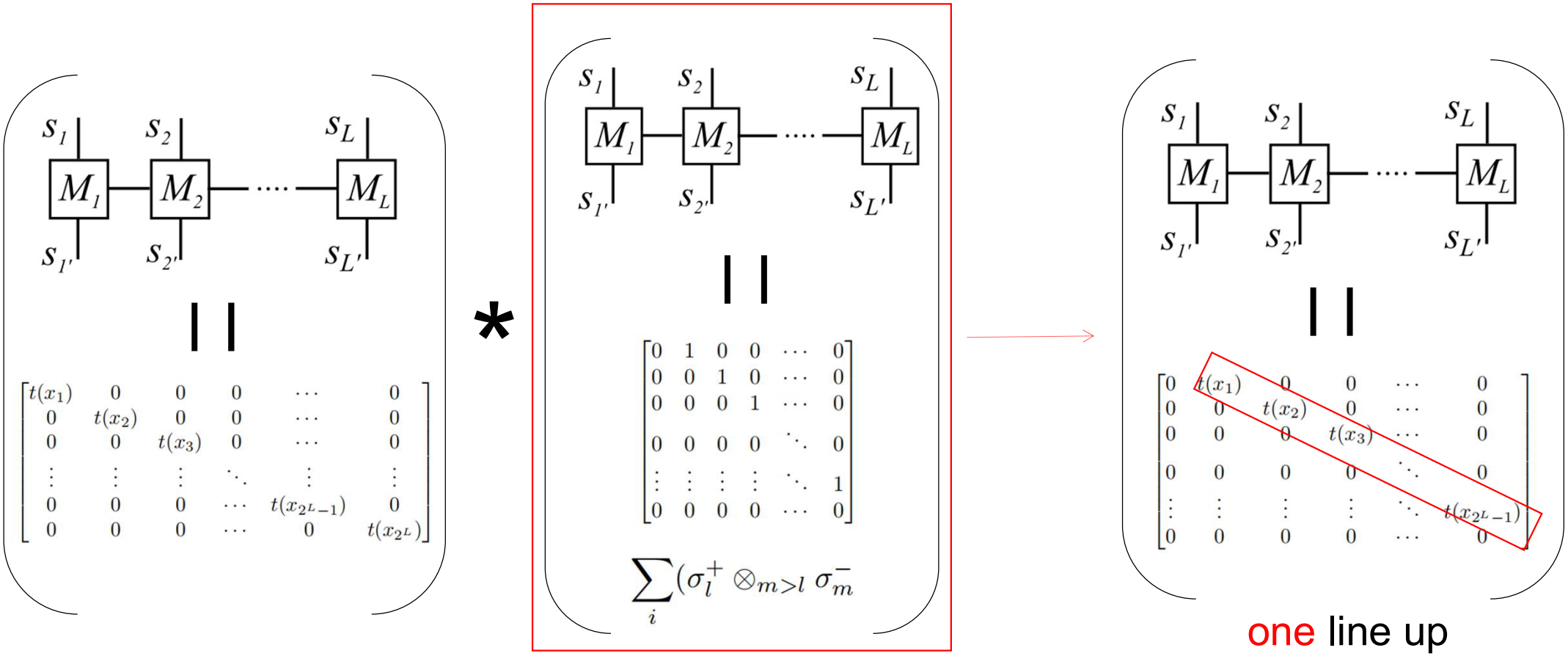
2. Inter-chain hopping:



Long-range hopping, hard to build?

A!

The shifting operator

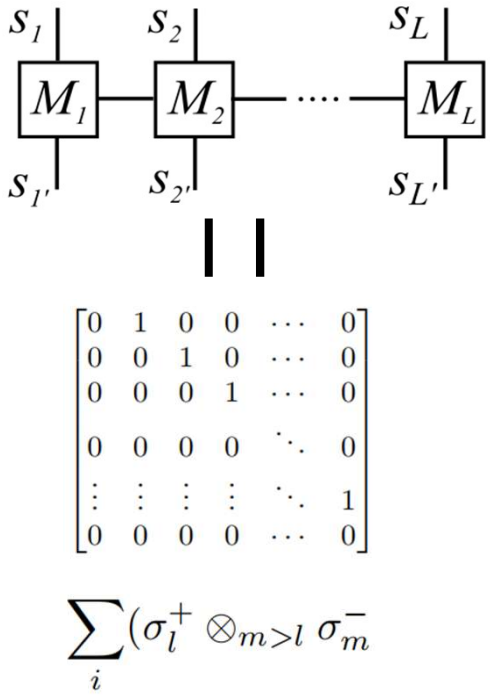


one line up

The shifting operator

A!

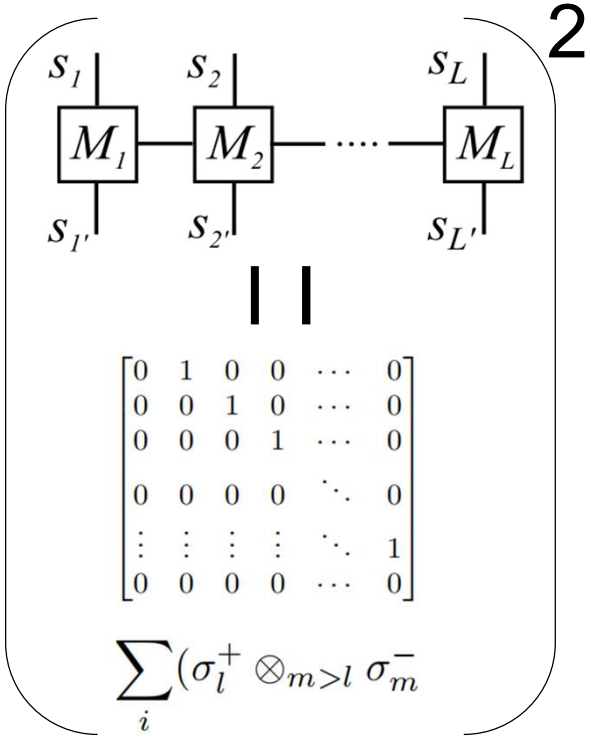
The exponential shifting operators



$$\begin{bmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 1 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \ddots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & 1 \\ 0 & 0 & 0 & 0 & \cdots & 0 \end{bmatrix}$$

$$\sum_i (\sigma_l^+ \otimes_{m>l} \sigma_m^-$$

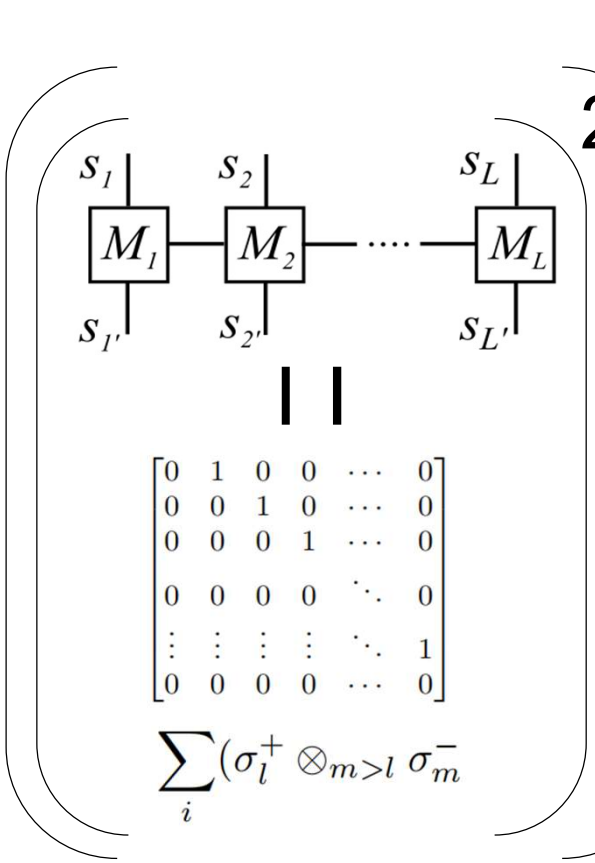
Shift elements one line up



$$\begin{bmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 1 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \ddots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & 1 \\ 0 & 0 & 0 & 0 & \cdots & 0 \end{bmatrix}$$

$$\sum_i (\sigma_l^+ \otimes_{m>l} \sigma_m^-$$

Shift elements two lines up



$$\begin{bmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 1 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \ddots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & 1 \\ 0 & 0 & 0 & 0 & \cdots & 0 \end{bmatrix}$$

$$\sum_i (\sigma_l^+ \otimes_{m>l} \sigma_m^-$$

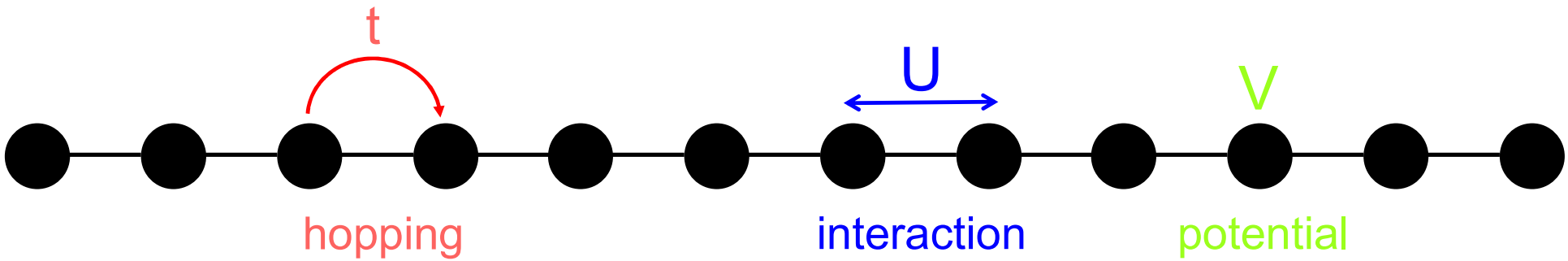
Shift elements four lines up

.....

A!

Easy realization of exponentially long ranging hopping operators

What about the interaction term?



$$H = \sum_{i,j} t(c_i c_j^\dagger + h.c.) + \sum_i V n_i + \boxed{\sum_{i,j} U n_i n_j}$$

?

A!

Aalto-yliopisto
Aalto-universitetet
Aalto University

Workflow of the mean-field algorithm

General idea of mean-field treatment

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

single-body term two-body term

Mean-field approximation: $$\sum_{\alpha\beta} V_{\alpha\beta} \langle c_\alpha^\dagger c_\alpha \rangle c_\beta^\dagger c_\beta + \ldots = \sum_{\alpha\beta} \chi_{\alpha\beta} c_\alpha^\dagger c_\beta$$

single-body term

Mean-field Hamiltonian: $$H^{MF} = \sum_{\alpha\beta} (t_{\alpha\beta} + \chi_{\alpha\beta}) c_\alpha^\dagger c_\beta = \sum_{\alpha\beta} H_{\alpha\beta}^{MF} c_\alpha^\dagger c_\beta$$

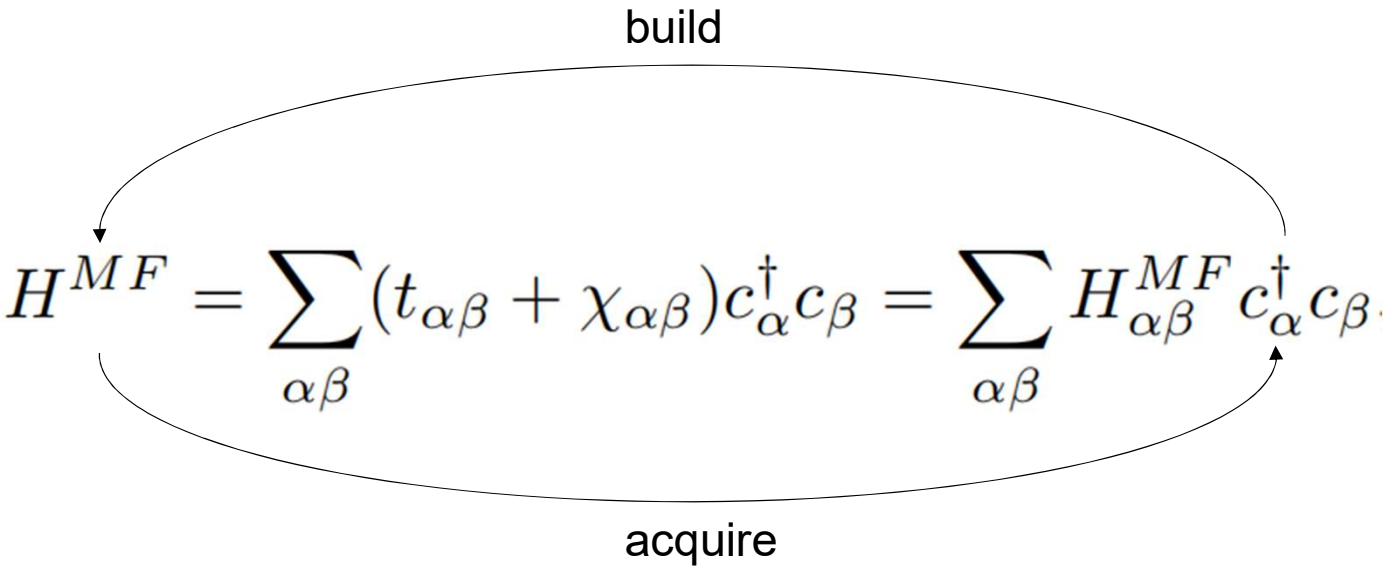
A!

Iterations of mean-field calculation

The goal: To get H^{MF} and $c_\alpha^\dagger c_\beta$

With initial guess of $\chi_{\alpha\beta}$:

The mean-field calculation:



Continue till convergence

A!

Model used in this research

Hubbard model:

$$H = \sum_{i,\sigma} t(c^{\dagger}_{i,\sigma} c_{i+1,\sigma} + h.c.) + \sum_{i} U(n_{i,\uparrow} - 1/2)(n_{i,\downarrow} - 1/2)$$

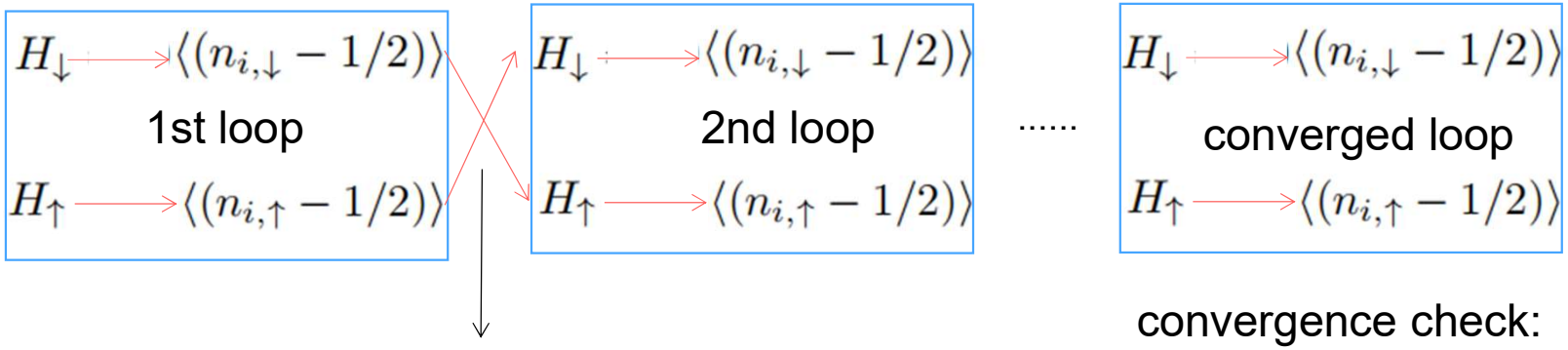
Mean-field Hamiltonian for 2 spins:

$$H_{\uparrow} = \sum_{i} t(c^{\dagger}_{i,\uparrow} c_{i+1,\uparrow} + h.c.) + \sum_{i} U(n_{i,\uparrow} - 1/2)\langle(n_{i,\downarrow} - 1/2)\rangle$$

$$H_{\downarrow} = \sum_{i} t(c^{\dagger}_{i,\uparrow} c_{i+1,\uparrow} + h.c.) + \sum_{i} U(n_{i,\downarrow} - 1/2)\langle(n_{i,\uparrow} - 1/2)\rangle$$

$\chi_{\alpha\beta}$

With initial guesses of electron densities :



mixing: $\langle n\rangle_{mix} = v\langle n\rangle_{new} + (1-v)\langle n\rangle_{old}$

convergence check:

$$|\langle n\rangle_{mix} - \langle n\rangle_{old}| < \epsilon$$

A!

Kernel polynomial method (KPM)

Suppose f(x) is defined on (-1,1):

$$f(x) = \frac{1}{\pi\sqrt{1-x^2}}\left[\mu_0 + 2\sum_{n=1}^{\infty}\mu_n T_n(x)\right]$$

The KPM expansion

Chebyshev polynomials:

$$T_n(x) = \cos[n \arccos(x)]$$

Chebyshev moments:

$$\mu_n = \int_{-1}^{1} f(x)\,T_n(x)\,dx$$

A!

Weiße A, Wellein G, Alvermann A, et al. The kernel polynomial method[J]. Reviews of modern physics, 2006, 78(1): 275-306.

Application of KPM in the mean-field calculation

Local density of state (LDOS) at energy ω and site i:

$$\cos[n \arccos(\omega)]$$

$$D_i(\omega) = \langle i|\delta(\omega - \tilde{H}_{MF})|i\rangle = \frac{1}{\pi\sqrt{1-\omega^2}}\langle i| \left[T_0(\tilde{H}_{MF}) + 2\sum_{n=1}^{\infty} T_n(\tilde{H}_{MF}) T_n(\omega)\right] |i\rangle$$

Electron density at site i:

$$\langle n_i\rangle = \int_{-\infty}^{\epsilon_F} D_i(\omega) d\omega \longrightarrow \langle n_i\rangle = 1 - \frac{1}{\pi}\langle i| \left[T_0(\tilde{H}_{MF})\cos(\epsilon_F) + 2\sum_{n=1}^{\infty} T_n(\tilde{H}_{MF}) \sin(n \arccos(\epsilon_F))\right] |i\rangle$$

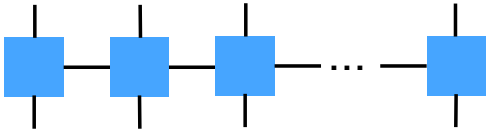
Chebyshev polynomials of Hamiltonian?

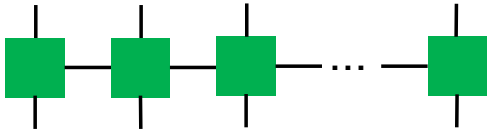
A!

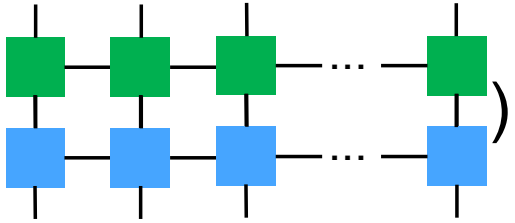
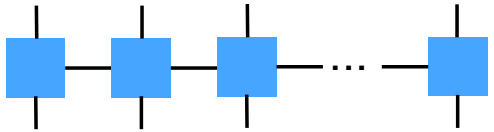
Chebyshev polynomials of Hamiltonian MPOs

The Chebyshev recursion relation:

$$T_0(\tilde{H}_{MF}) = I$$
$$T_1(\tilde{H}_{MF}) = \tilde{H}_{MF}$$
$$T_{n+1}(\tilde{H}_{MF}) = 2\tilde{H}_{MF}T_n(\tilde{H}_{MF}) - T_{n-1}(\tilde{H}_{MF})$$

In our case: $T_0(\tilde{H}_{MF}) =$  Identity MPO

$T_1(\tilde{H}_{MF}) =$  Hamiltonian MPO

$T_2(\tilde{H}_{MF}) = 2($  $) -$ 

.....

Easy realization with contraction & summation

A!

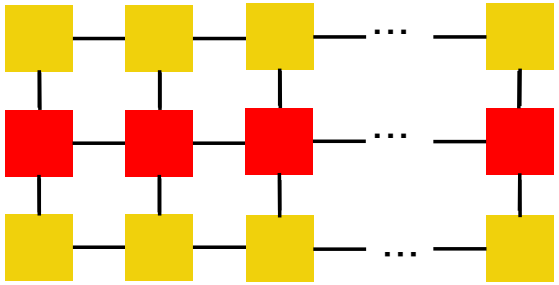
Acquiration of electron density

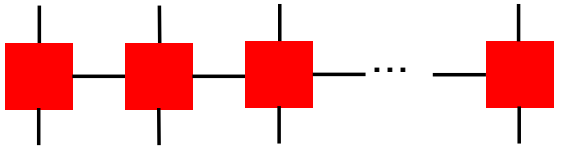
Electron density at site i:

$$\langle n_i \rangle = 1 - \frac{1}{\pi}\langle i| \left[T_0(\tilde{H}_{MF}) \arccos(\epsilon_F) + \frac{2}{n}\sum_{n=1}^{\infty} T_n(\tilde{H}_{MF}) \sin(n \arccos(\epsilon_F)) \right] |i\rangle$$

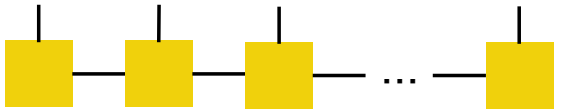
$$= 1 - \langle i|A|i\rangle$$

With tensor networks:

$\langle n_i \rangle =$ 



: The MPO “A”



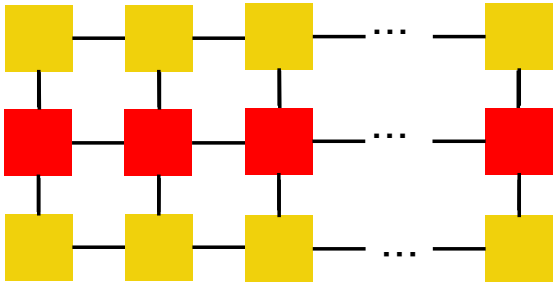
: The state vector MPS for site i

Do we need to do it for all sites?

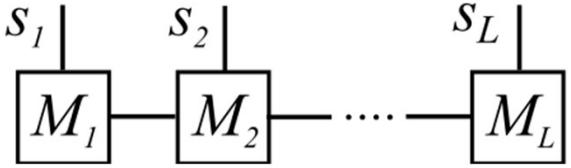
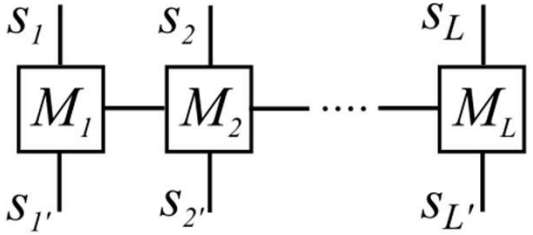
A!

Acquiration of electron density with QTCI

$$\langle n_i \rangle = 1 - \langle i|A|i\rangle =$$



A function of i!

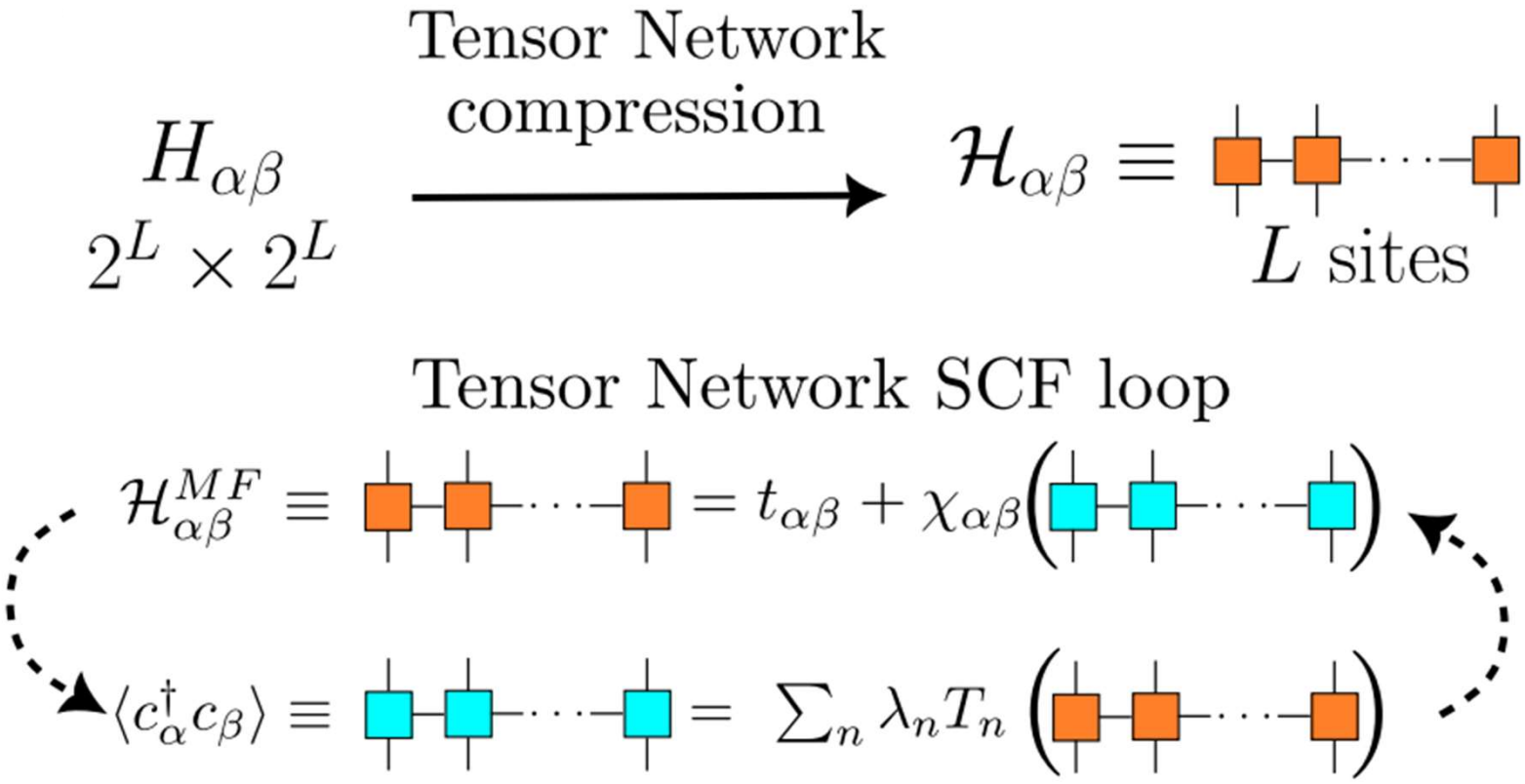
$1 - \langle i|A|i\rangle$ → QTCI →  → diagonal MPO → 

diagonal MPO for the electron densities

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

A!

Summarized workflow of tensor network mean-field calculation

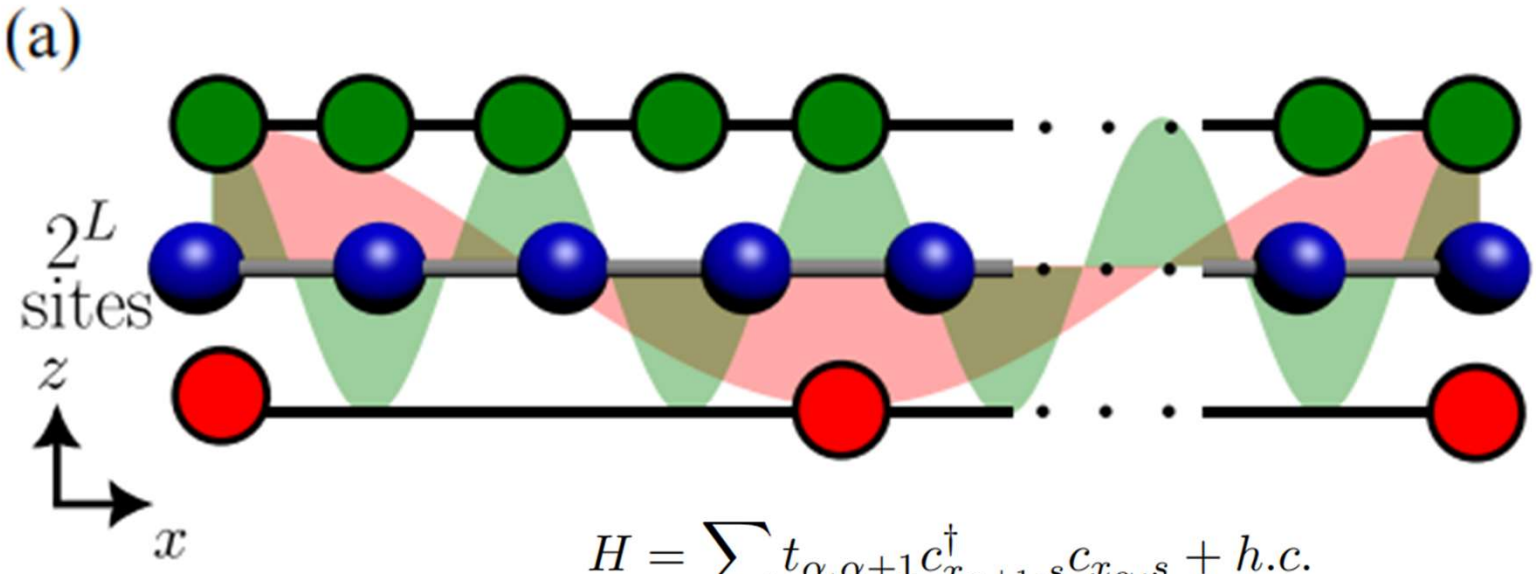


A!

Aalto-yliopisto
Aalto-universitetet
Aalto University

Results & summary

One-dimensional super-moiré system



$$H = \sum_{\alpha,s} t_{\alpha,\alpha+1} c^{\dagger}_{x_{\alpha+1},s} c_{x_\alpha,s} + h.c.$$

$$+ \sum_{\alpha} U_\alpha \left(c^{\dagger}_{x_\alpha,\uparrow} c_{x_\alpha,\uparrow} - \frac{1}{2} \right) \left(c^{\dagger}_{x_\alpha,\downarrow} c_{x_\alpha,\downarrow} - \frac{1}{2} \right)$$

L = 30

$$|\langle n \rangle_{mix} - \langle n \rangle_{old}| < \epsilon$$ criteria as 10^{-3}

A! beyond 1 billion sites

Results for the one-dimensional super-moiré system

A super-moiré hopping term:

$$t(X_\alpha) = t_0 + t_1\cos(k_1 X_\alpha) + t_2\cos(k_2 X_\alpha)$$

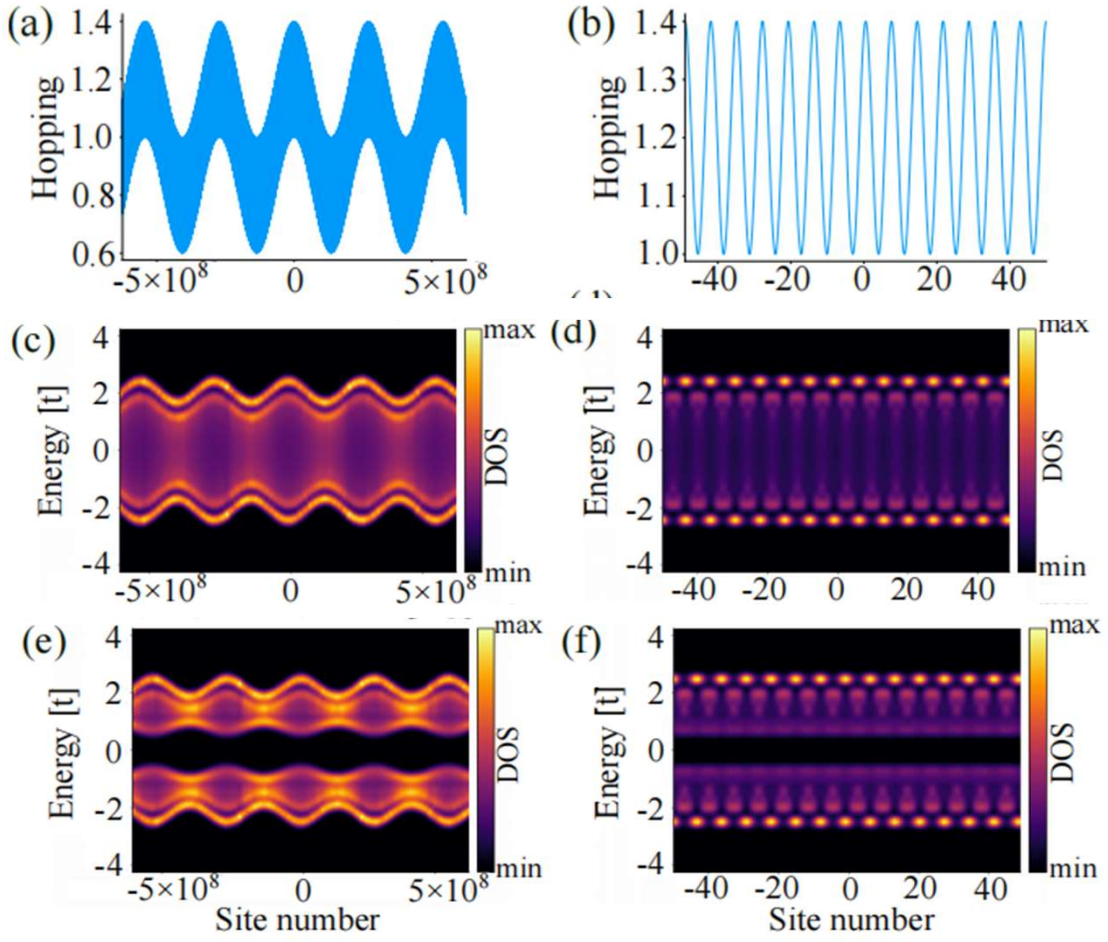
$$X_\alpha = \frac{x_\alpha + x_{\alpha+1}}{2}$$

$$k_1 = \frac{2\pi}{5\sqrt{2}} \text{ and } k_2 = \frac{8\pi}{2^{29}\sqrt{3}}$$

Results of LDOS
with/without interaction:

Time consumption:
~40000 seconds/11 hours
on a single core of CPU

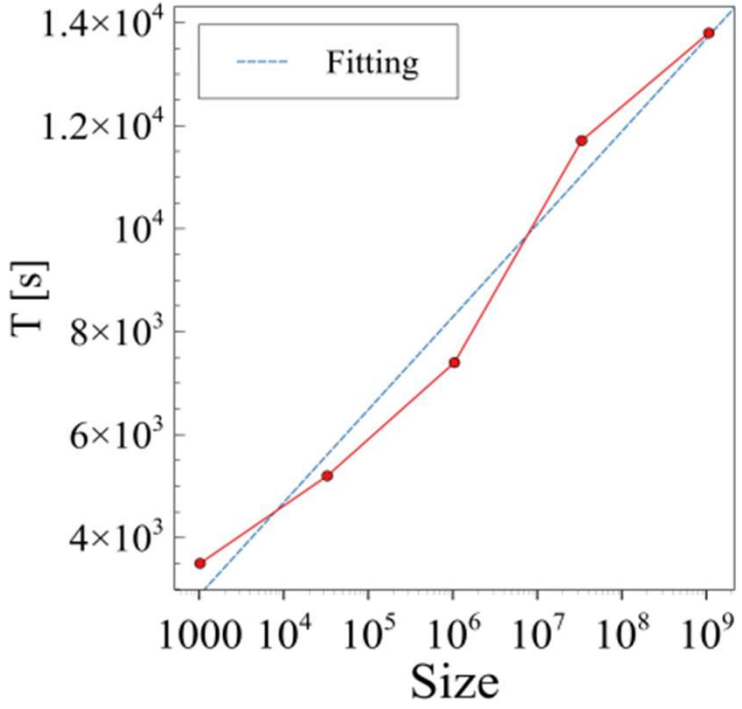
The modulation:



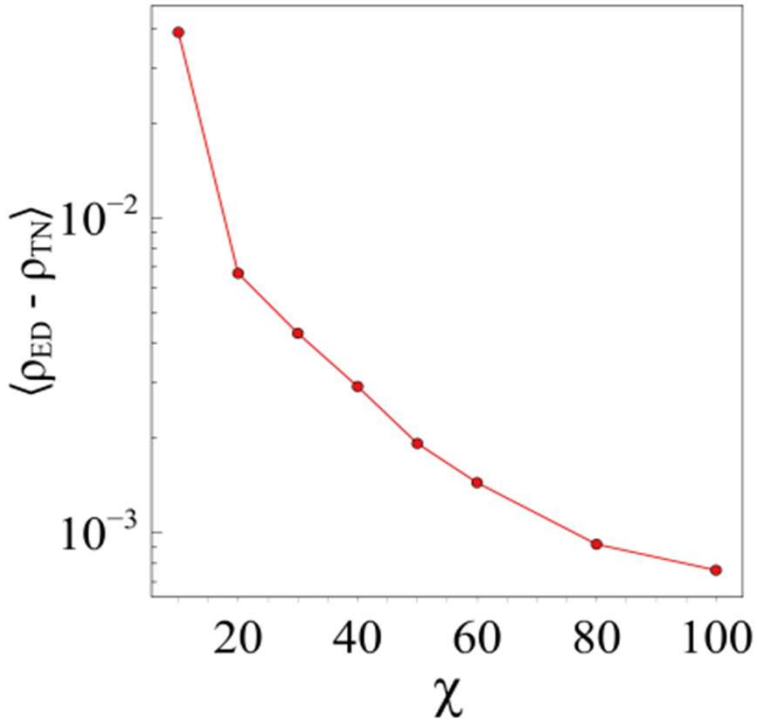
A!

The accuracy and efficiency benchmarking

With 10 rounds of mean-field iterations:



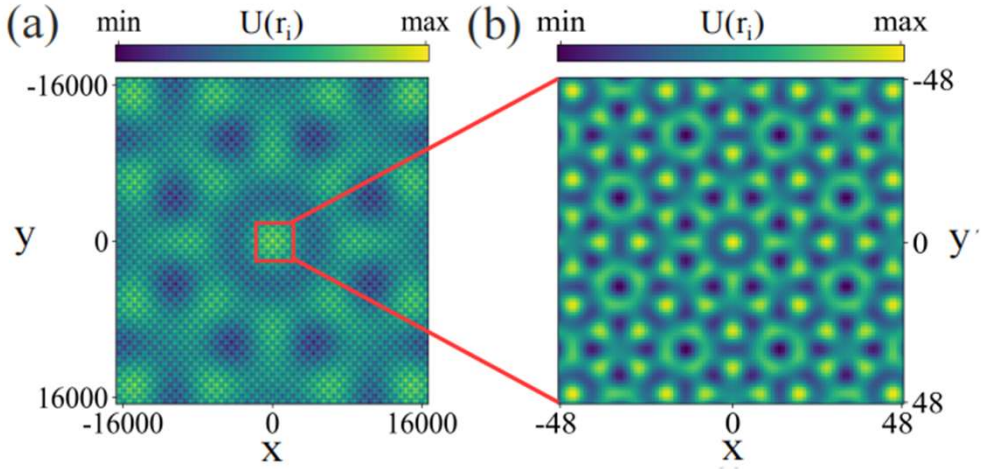
Comparison with exact diagonalization:



Results for the super-moiré square quasi-crystal

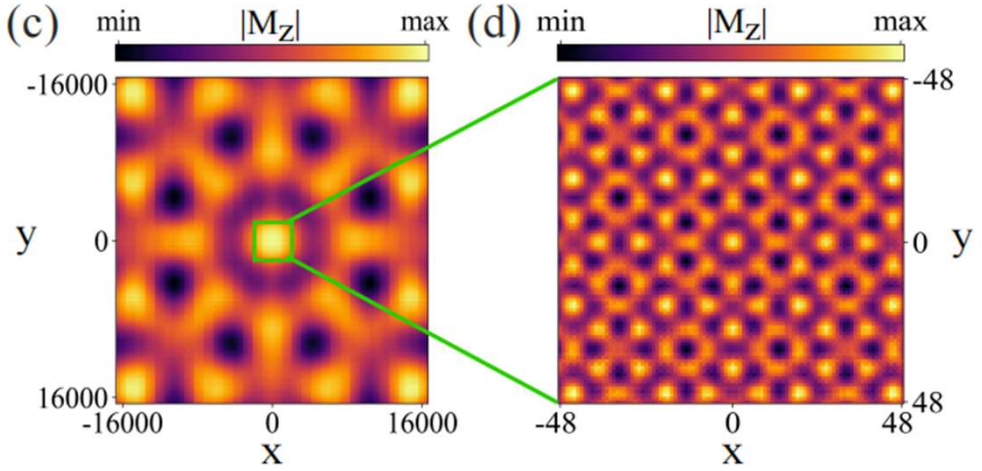
A super-moiré 8-fold interaction term: $U(r_i) = 8 + 0.5\{\sum_{i=1}^{4} \cos(k_1 \mathbf{n}_i \cdot \mathbf{r}_i) + \cos(k_2 \mathbf{n}_i \cdot \mathbf{r}_i)\}$

The interaction modulation:



The magnetization:

$$|M_z| = |n_\uparrow - n_\downarrow|$$



A!

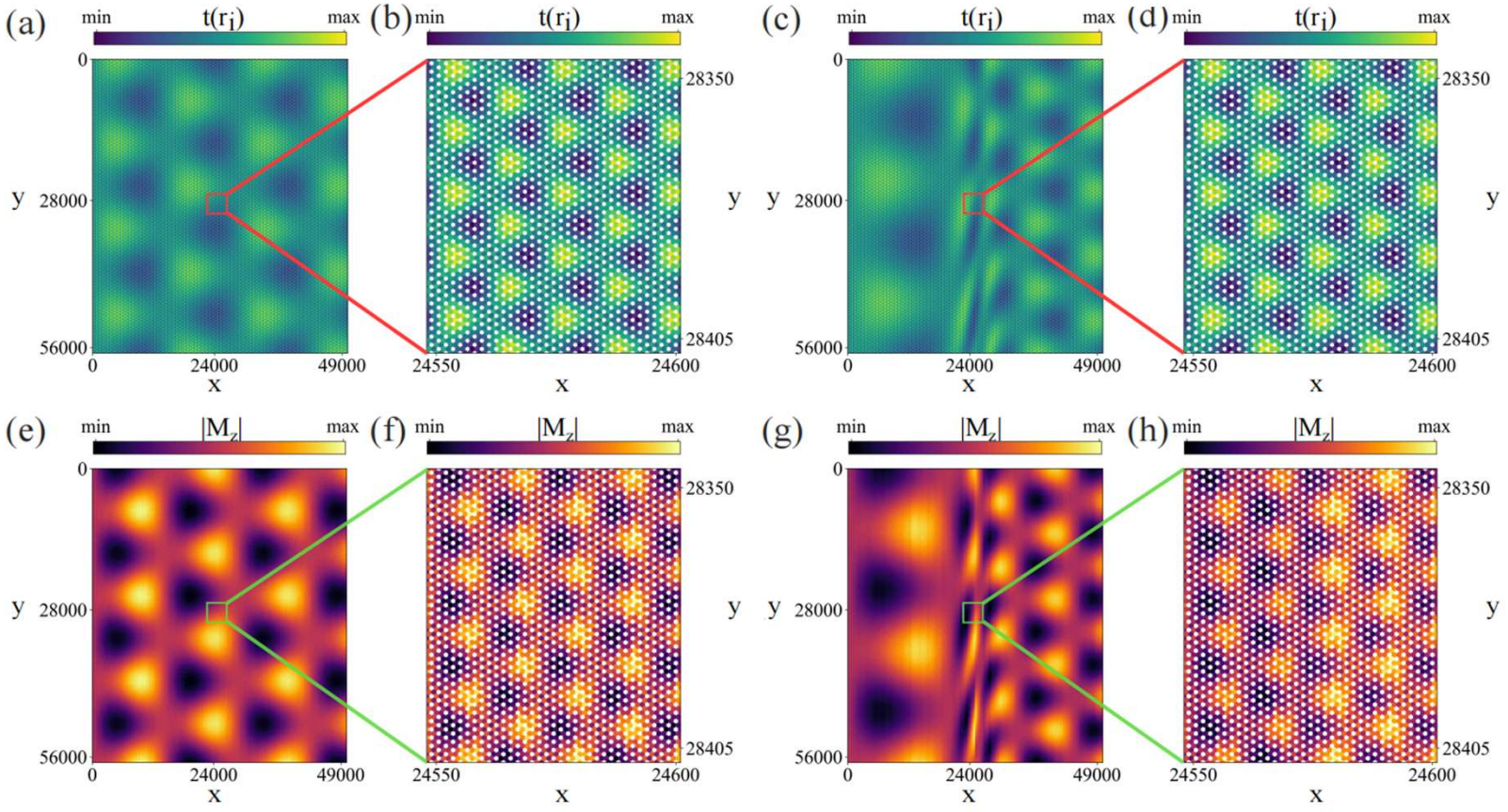
Results for super-moiré graphene with 2^{31} sites

$$t_{ij} = 1 + 0.2\sin(k_1 \mathbf{u}_{ij} \cdot \mathbf{R}_{ij}) + 0.2\sin(k_2 \mathbf{u}_{ij} \cdot \mathbf{R}_{ij})$$

$$\tilde{k}_1 = k_1\left(1 + \delta \tanh\left(\frac{\mathbf{u}_{ij} \cdot \mathbf{R}_{ij}}{W}\right)\right)$$

The modulation:

The magnetization:



A!

Plain super-moiré graphene

With domain wall

Summary

1. We have developed a general formalism for exponentially compressing most common 1D/2D tight-binding Hamiltonians into tensor network form using the QTCI algorithm.

2. Based on this formalism, further utilizing KPM method we have developed a general methodology for performing mean-field calculation for super-moiré systems with over one billion sites (or even more).

3. Both the formalism and the mean-field methodology could be widely applied in various fields, including superconductors, quasi-crystals, etc. (please check the posters!)

A!

References:

1. Cao Y, Fatemi V, Fang S, et al. Unconventional superconductivity in magic-angle graphene superlattices[J]. Nature, 2018, 556(7699): 43-50.

2. Li H, Xiang Z, Naik M H, et al. Imaging moiré excited states with photocurrent tunnelling microscopy[J]. Nature materials, 2024, 23(5): 633-638.

3. Cai J, Anderson E, Wang C, et al. Signatures of fractional quantum anomalous Hall states in twisted MoTe2[J]. Nature, 2023, 622(7981): 63-68

4. Andrei E Y, Efetov D K, Jarillo-Herrero P, et al. The marvels of moiré materials[J]. Nature Reviews Materials, 2021, 6(3): 201-206.

5. Sun Y, Niedermeier M, Antão T V C, et al. Self-consistent tensor network method for correlated super-moir\'e matter beyond one billion sites[J]. arXiv preprint arXiv:2503.04373, 2025.

6. Núñez Fernández Y, Ritter M K, Jeannin M, et al. Learning tensor networks with tensor cross interpolation: new algorithms and libraries[J]. SciPost Physics, 2025, 18(3): 104.

7. Weiße A, Wellein G, Alvermann A, et al. The kernel polynomial method[J]. Reviews of modern physics, 2006, 78(1): 275-306.

A!

The work

Condensed Matter > Strongly Correlated Electrons

[Submitted on 6 Mar 2025]

Self-consistent tensor network method for correlated super-moiré matter beyond one billion sites

Yitao Sun, Marcel Niedermeier, Tiago V. C. Antão, Adolfo O. Fumega, Jose L. Lado

Moiré and super-moiré materials provide exceptional platforms to engineer exotic correlated quantum matter. The vast number of sites required to model moiré systems in real space remains a formidable challenge due to the immense computational resources required. Super-moiré materials push this requirement to the limit, where millions or even billions of sites need to be considered, a requirement beyond the capabilities of conventional methods for interacting systems. Here, we establish a methodology that allows solving correlated states in systems reaching a billion sites, that exploits tensor-network representations of real-space Hamiltonians and self-consistent real-space mean-field equations. Our method combines a tensor-network kernel polynomial method with quantics tensor cross interpolation algorithm, enabling us to solve exponentially large models, including those whose single particle Hamiltonian is too large to be stored explicitly. We demonstrate our methodology with super-moiré systems featuring spatially modulated hoppings, many-body interactions and domain walls, showing that it allows access to self-consistent symmetry broken states and spectral functions of real-space models reaching a billion sites. Our methodology provides a strategy to solve exceptionally large interacting problems, providing a widely applicable strategy to compute correlated super-moiré quantum matter.

A!