Aalto University Department of Applied Physics

**PHYS-EV0007 — Machine Learning from and for Quantum Science**

Topic: Simulating a large interacting tight-binding model with moiré potentials using tensor networks

*Based on* Y. Sun et al., Phys. Rev. Res. **7**, 043288 (2025)

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**Topic nr 1**
**Project nr 1**

## Project description

Understand and apply tensor-network–based methods (KPM combined with quantics tensor cross-interpolation QTCI) to compute self-consistent correlated states and spectral functions of ultra-large nonperiodic tight-binding models.

## Learning outcomes

- Understand tight-binding modeling of nonperiodic systems using tensor networks and apply it to mean-field correlated states.
- Gain working knowledge of Tensor Cross Interpolation (TCI) and the Quantics/Quantics-TCI methods.
- Understand the Kernel Polynomial Method (KPM) in a tensor-network setting and its scaling properties.

## Presentation

- Explain the formalism used in the paper:
  - Tight-Binding, Pseudo-Spin Encoding, KPM Spectral Methods, Mean-Field
- Explain how QTCI is incorporated into this framework.
- Explain the advantages and limitations of the method.

## Simulations

### Warm up questions

1. Consider the function

$$f(x) \;=\; e^{-20\,(x-\frac{1}{3})^2}\cos(10\pi x) \;+\; e^{-40\,(x-\frac{2}{3})^2}\sin(20\pi x) \;+\; \tfrac{1}{4}\cos(2\pi x), \qquad x\in[0,1], \quad (1)$$

   Use QTCI to approximate it.

a. Plot both the exact function and its quantics tensor train approximation.

b. Plot the bond dimension across the tensor train and extract the error in the approximation.

c. Plot the rank (maximum bond dimension) as a function of bit-depth $R \in \{6, 8, 10, \ldots, 24\}$.

2. Consider the Weierstrass function, truncated at analytic depth $D$,

$$W_D(x) \;=\; \sum_{n=0}^{D} a^{\,n} \cos(b^{\,n}\pi x)\,, \qquad x \in [0,1], \tag{2}$$

with the two parameter sets

$$(a,b)_1 = \left(\tfrac{1}{2},\, 13\right), \qquad (a,b)_2 = \left(\tfrac{7}{10},\, 9\right),$$

both of which satisfy $0 < a < 1$, $b \in \mathbb{Z}_+^{\text{odd}}$, and $ab > 1 + \frac{3\pi}{2}$. The analytic tail is bounded by

$$\varepsilon_D^{\text{trunc}} \;\equiv\; \|W - W_D\|_\infty \;\le\; \frac{a^{D+1}}{1-a}. \tag{3}$$

Use QTCI to approximate $W_D$ on a bit-depth-$R$ grid $x_k = k/2^R,\ k = 0, \ldots, 2^R - 1$, and for *each* parameter set:

a. Plot $W_D(x)$ and its quantics tensor-train approximation $W_D^{\text{QTCI}}(x)$ for a representative $(D, R)$.

b. Plot the bond dimension along the tensor train and extract the QTCI error $\varepsilon_{D,R}^{\text{QTCI}} = \|W_D - W_D^{\text{QTCI}}\|_\infty$.

c. Plot the rank (maximum bond dimension) $\chi_{\max}$ as a function of bit-depth $R$, at fixed $D$.

d. **Analytic vs. QTCI error.** On a single log-scale figure, overlay

$$\varepsilon_D^{\text{trunc}} \quad \text{(analytic bound, Eq. 3)} \qquad \text{and} \qquad \varepsilon_{D,R}^{\text{QTCI}} \quad \text{(numerical)}$$

as functions of $D$, at fixed $R$ large enough to resolve the highest frequency $b^D$ (i.e. $2^R \gtrsim b^D$).

e. Is this function compressible? Using the observed scaling $\chi_{\max}(R)$ and the comparison above, explain why the two parameter sets compress differently, and relate your answer to the Hölder exponent $\alpha = -\log a / \log b$.

**Simulation of an interacting Hamiltonian**

1. Construct a matrix-product-operator (MPO) representation of a 1D tight-binding chain Hamiltonian

$$H \;=\; -\sum_i t(x_i)(c_i^\dagger c_{i+1} + \text{h.c.}), \qquad t(x_i) = t_0 \cos\!\left(2\pi x_i/\sqrt{3}\right), \tag{4}$$

Work on a chain of size $N = 2^R$ with $R$ large enough to be non-trivial but reasonable on your machine.

a. What is its bond-dimension as a function of system size?

b. Is it a compressible Hamiltonian? Explain your reasoning.

2. With the same Hamiltonian, consider an incommensurate interaction potential between electrons of the form

$$U(x) = U_0 \left[ \sin\left(\frac{2\pi x}{\sqrt{2}}\right) + \sin\left(\frac{2\pi x}{\sqrt{5}N}\right) \right], \tag{5}$$

   a. Perform a mean-field decoupling using the SCF algorithm found in the paper with $N_\mu = 50$ moments. How many iterations are needed for convergence?

   b. What is the bond-dimension of the final Hamiltonian?

   c. Calculate the local density of states across the chain. What is the difference with respect to the non-interacting case?

   d. Calculate the magnetization as a function of lattice position across the chain.

3. Perform a numerical benchmarking analysis.

   a. Calculate the convergence time of the SCF solution for a few system sizes.

   b. Calculate the convergence time of the SCF solution for a few different number of Chebyshev moments.

   c. Calculate the convergence error as a function of number of Chebyshev moments for a few system sizes.

## Deliverables

- A concise report on the article in the form of a presentation.
- A repo with organized, well-documented code, and a notebook with working examples for the simulations.

## Working practices and tools

*You are strongly encouraged to recycle existing material.* You are expected to **read, reuse, and adapt** existing reference implementations pipelines rather than re-derive or re-implement every algorithmic detail from scratch; the pedagogical goal of this project is to *understand and apply* the method, not to reproduce boilerplate. Any code you borrow must be clearly attributed in your repository (e.g. in a `README.md` or as in-source comments) and integrated cleanly with your own contributions. *Use of LLMs (ChatGPT, Claude, Gemini, . . . ) is permitted and encouraged for onboarding.* In particular, LLMs are very effective at:

- explaining unfamiliar programming syntax and idioms;
- summarising sections of the paper or cross-referencing related literature;
- debugging installation issues, bookkeeping, and programming recommendations;
- generating boilerplate (plotting scripts, parameter sweeps, unit tests, diagnostic helpers).

You remain, however, fully responsible for the correctness, clarity, and scientific content of what you submit: LLM output must be checked, understood, and, where appropriate, cited. Treat an LLM as a capable but occasionally wrong collaborator, not as an oracle.

**Programming language:** Julia.

**Packages required:** ITensor, ITensorMPS, TCI, QTCI.

## References


- Y. Sun et al., Phys. Rev. Res. **7**, 043288 (2025).
- Y. Sun Github repo for the paper (2025)
- Y. Núñez Fernández et al., SciPost Phys. **18**, 104 (2025).
- X. Waintal et al., arXiv 2601.03035 (2026).