PHYS-EV0007 — Machine Learning from and for Quantum Science

Topic: Real-space topology using tensor networks algorithms
for local topological markers

Based on T. V. C. Antão et al., Phys. Rev. Lett. **136**, 156601 (2026)

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Topic nr 1
Project nr 2

Project description

Understand and apply tensor-network–based methods (quantics tensor cross-interpolation QTCI, the Chebyshev/Kernel-Polynomial tensor-network representation of the density matrix, and real-space local topological markers) to characterize the topology of ultra-large nonperiodic tight-binding models.

Learning outcomes

- Understand tight-binding modeling of nonperiodic systems using tensor networks and the calculation of real-space local topological markers from the tensor-network density matrix.
- Gain working knowledge of Tensor Cross Interpolation (TCI) and the Quantics/Quantics-TCI methods for *both* smooth and integer-lattice functions.
- 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, Chebyshev / KPM tensor-network representation of the density matrix, local topological markers, Chern mosaics in quasicrystals.
- Explain how QTCI is incorporated into this framework.
- Explain the advantages and limitations of the method.

Simulations

Warm up questions

1. Consider the multi-scale function

$$f(x) \;=\; \frac{\sin(12\pi x)}{1 + 50\,(x - \frac{1}{2})^2} \;+\; \tfrac{1}{4}\tanh\!\big(8\,(x - \tfrac{1}{3})\big)\,\cos(20\pi x), \qquad x \in [0,1], \tag{1}$$

Use QTCI to approximate it.

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

b. Plot the bond dimension along the tensor train and extract the approximation error $\varepsilon_R = \|f - f^{\mathrm{QTCI}}\|_\infty$.

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

2. Consider the **silver mean substitution sequence** on the integer lattice, defined by the two-letter substitution $\sigma: A \mapsto AAB,\ B \mapsto A$ iterated from the seed A, with the letter-to-value map $A \mapsto -1,\ B \mapsto +1$. The first few terms are

$$v_n = -1,\ -1,\ +1,\ -1,\ -1,\ +1,\ -1,\ -1,\ -1,\ -1,\ +1,\ \ldots \qquad n = 0, 1, 2, \ldots \tag{2}$$

Equivalently, v_n admits the closed-form cut-and-project expression

$$v_n = \operatorname{sgn}\Big(\cos\!\big(2\pi\,(\sqrt{2}-1)\,(n+1)\big) - \cos\!\big(\pi\,(\sqrt{2}-1)\big)\Big), \tag{3}$$

which is convenient for numerical evaluation at arbitrary n. Define the integer-indexed sequence on $n \in \{0, 1, \ldots, 2^R - 1\}$ and use QTCI to approximate it directly (*no* continuous interpolation: treat n as a binary-encoded integer coordinate).

a. Plot both the exact sequence v_n and its quantics tensor-train approximation v_n^{QTCI} for, e.g., $R = 16$.

b. Plot the bond dimension along the tensor train and extract the approximation error $\varepsilon_R = \max_n |v_n - v_n^{\mathrm{QTCI}}|$.

c. Plot the maximum rank $\chi_{\max}$ as a function of R for $R \in \{6, 8, \ldots, 24\}$. Comment on the scaling.

d. Is the silver mean sequence compressible? Relate your observed scaling to the self-similar structure of the sequence, and contrast it with (i) a fully periodic ± 1 sequence and (ii) a random Bernoulli ± 1 sequence (generically incompressible).

Simulation of a modulated SSH chain

1. **Building the Hamiltonian.** Construct a matrix-product-operator (MPO) representation of the 1D modulated SSH Hamiltonian

$$H = -\sum_i t_i\,(c_i^\dagger c_{i+1} + \text{h.c.}), \qquad t_i = t + (-1)^i\,\delta_i, \qquad \delta_i = d\,\cos\!\Big(\tfrac{2\pi\,i}{\lambda}\Big), \tag{4}$$

with constant mean hopping t, dimerization amplitude d, and spatial modulation wavelength λ. The uniform case is recovered for d constant in space, i.e. $\lambda \to \infty$ (equivalently, replace $\delta_i \to d$ everywhere). 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 the bond-dimension of the Hamiltonian MPO as a function of system size N (uniform and modulated cases)?

b. Is this a compressible Hamiltonian? Explain your reasoning in terms of the quantics ranks of the staggering $(-1)^i$ and the modulation $\cos(2\pi i/\lambda)$.

2. **Local topological marker (no modulation).** Construct the real-space local marker

$$\mathcal{W} = P\,X\,Q + Q\,X\,P, \qquad P = \sum_{E_n < E_F} |\psi_n\rangle\langle\psi_n|\,, \quad Q = \mathbb{1} - P, \tag{5}$$

where $X = \mathrm{diag}(1, 2, \ldots, N/2) \otimes \mathbb{1}_{2\times 2}$. This operator is written to represent the position of a 2-site unit cell. Note that you should regularize this operator in a similar way as is done in the paper. P projects on the occupied subspace (half-filling, $E_F = 0$ for the SSH model). The local marker is the site-diagonal element $\mathcal{W}(i) \equiv \langle i| \mathcal{W} |i\rangle$; this is the 1D analogue of the real-space Chern markers used in the paper (see also arXiv:2209.10703 for the generic local-marker framework). First, set d uniform in space, and compute $\mathcal{W}(i)$ using the KPM machinery of the paper.

   a. Plot the spatially averaged marker $\bar{\mathcal{W}} = N^{-1} \sum_i \mathcal{W}(i)$ as a function of $d \in [-t, +t]$. Identify the topological transition and verify that $\bar{\mathcal{W}}$ takes distinct (approximately quantized) values on the two sides.

3. **Local density of states and edge modes.** For a small system $N = 2^5$, compute the local density of states $\rho(i, \omega)$ using the KPM / Chebyshev tensor-network machinery of the paper with N_μ Chebyshev moments.

   a. For uniform $d < 0$ and uniform $d > 0$, plot $\rho(i, \omega)$ as a heatmap on the (i, ω) plane. Identify the zero-energy boundary modes in the topological phase and their absence in the trivial phase.

   b. Extract the spatial profile $\rho(i, \omega\!=\!0)$ of the zero-energy boundary modes; verify the expected exponential localization at the chain ends.

4. **Local winding number in a modulated chain (topological mosaic).** Re-introduce the spatial modulation $\delta_i = d \cos(2\pi i/\lambda)$ with λ chosen so that the chain contains several "domains" of alternating topology (e.g. $\lambda \sim N/4$).

   a. Plot $\mathcal{W}(i)$ across the chain. Identify the spatial "mosaic" of topologically non-trivial and trivial regions.

   b. Overlay the plot with the sign of the local dimerization $\mathrm{sgn}(\delta_i)$ and comment on the correspondence between sign changes of δ_i and interfaces in $\mathcal{W}(i)$.

5. **Performance benchmarking.** Carry out a systematic numerical benchmarking of the full pipeline (MPO assembly + Chebyshev / KPM recursion + local-marker evaluation).

   a. Measure the wall-clock time for computing $\mathcal{W}(i)$ as a function of system size $N = 2^R$ for $R \in \{5, \ldots, R_{\max}\}$, with $R_{\max}$ chosen as the largest size that fits comfortably on your machine. Plot time vs. R on a log-log axis and extract the effective scaling exponent.

   b. Measure the wall-clock time as a function of the number of Chebyshev moments N_μ at fixed R.

   c. Measure the convergence error of the local marker (e.g. $\|\mathcal{W}^{(N_\mu)} - \mathcal{W}^{(N_\mu^{\max})}\|_2$ on a reference grid) as a function of N_μ, for a few system sizes.

   d. Report the peak bond dimension reached during the Chebyshev / KPM recursion and during the assembly of $\mathcal{W}$.

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

- T. V. C. Antão et al., Phys. Rev. Lett. **136**, 156601 (2026).
- T. V. C. Antão, GitHub repo for the paper (2026).
- *Generic local topological markers*: arXiv:2209.10703.
- Y. Núñez Fernández et al., SciPost Phys. **18**, 104 (2025).
- X. Waintal et al., arXiv:2601.03035 (2026).