Aalto University Department of Applied Physics

PHYS-EV0007 — Machine Learning from and for Quantum Science

Topic: Momentum-resolved spectral functions of quasi-periodic tight-binding models using tensor networks

Based on A. Moustaj et al., arXiv:2512.18397 (2025)

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Topic nr 1
Project nr 3

Project description

Understand and apply tensor-network–based methods (quantics tensor cross-interpolation QTCI, the Kernel Polynomial Method KPM, and the MPO formulation of the quantum Fourier transform QFT) to compute local and momentum-resolved spectral functions of ultra-large nonperiodic tight-binding models.

Learning outcomes

- Understand tight-binding modeling of nonperiodic systems using tensor networks and apply quantum Fourier transforms to extract momentum space data.
- 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, Pseudo-Spin Encoding, KPM Spectral Methods, Fourier Transform representation
- Explain how QTCI is incorporated into this framework.
- Explain the advantages and limitations of the method.

Simulations

Warm up questions

1. Consider the golden-ratio–modulated, Gaussian-enveloped function

$$f(x) \;=\; e^{-10\,(x-\frac{1}{2})^2}\Big[\cos(2\pi x) \;+\; \cos(2\pi\,\varphi\,x)\Big] \;+\; \tfrac{1}{4}\,\mathrm{sech}\big(8\,(x-\tfrac{1}{3})\big), \qquad x\in[0,1], \tag{1}$$

with $\varphi = (1+\sqrt{5})/2$ the golden ratio. 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 **Fibonacci substitution sequence** on the integer lattice, defined by the two-letter substitution $\sigma : A \mapsto AB,\ B \mapsto A$ iterated from the seed A, with the letter-to-value map $A \mapsto -1,\ B \mapsto +1$. The first few terms are

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

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

$$v_n \;=\; \mathrm{sgn}\Big(\cos\!\big(2\pi\,\varphi^{-1}\,(n+1)\big) \;-\; \cos\!\big(\pi\,\varphi^{-1}\big)\Big), \qquad \varphi = \tfrac{1+\sqrt{5}}{2}, \tag{3}$$

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 Fibonacci 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 quasi-periodic tight-binding chain

1. **Building the Hamiltonian** Construct a matrix-product-operator (MPO) representation of the 1D Aubry–André–Harper (AAH) Hamiltonian

$$H \;=\; -t \sum_i (c_i^\dagger c_{i+1} + \mathrm{h.c.}) \;+\; \sum_i V_i\, c_i^\dagger c_i, \qquad V_i \;=\; V \cos\!\big(2\pi\beta\, i\big), \tag{4}$$

with constant hopping t, quasi-periodic modulation strength V, incommensurate wavenumber $\beta = \varphi^{-1}$ (golden ratio) and an arbitrary phase ϕ. 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. **Local density of states**. Using the KPM machinery of the paper with N_μ Chebyshev moments (reasonable number for your machine), compute the local density of states $\rho(i, \omega)$.

a. Choose at least three regimes: $V/t < 2$ (delocalized), $V/t = 2$ (AAH critical point), $V/t > 2$ (localized). Plot $\rho(i, \omega)$ as a heatmap on the (i, ω) plane for each regime.

b. Comment on the qualitative differences between the three regimes and relate them to the Aubry–André self-dual localization transition.

c. Plot the total density of states $\mathrm{Tr}\,\delta(\omega - \hat{H})$ and identify the characteristic fractal / Cantor-set-like features of the AAH spectrum.

3. **Momentum-resolved spectral function via MPO–QFT.** Construct the MPO representation of the quantum Fourier transform (QFT) $\hat{\mathcal{F}}$ acting on the quantics-encoded site index. Use it to compute the momentum-resolved spectral function

$$A(k,\omega) \;=\; \langle k|\,\hat{\mathcal{F}}\delta(\omega - \hat{H})\hat{\mathcal{F}}^{-1}\,|k\rangle\,. \tag{5}$$

   a. For each of the three regimes of the previous item, plot $A(k,\omega)$ as a heatmap on the (k,ω) plane.

   b. Discuss the spectral-weight distribution across k in the delocalized, critical, and localized regimes.

4. **Performance benchmarking.** Carry out a systematic numerical benchmarking of the full pipeline (MPO assembly + KPM moments + MPO–QFT).

   a. Measure the wall-clock time for computing $\{\rho_i(\omega)\}$ and $A(k,\omega)$ as a function of system size $N = 2^R$ for $R \in \{5,\ldots,R_{\max}\}$ with $R_{\max}$ is 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 at fixed R.

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

   d. Report the peak bond dimension reached during the QFT step and the KPM recursion.

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

- A. Moustaj et al., arXiv:2512.18397 (2025).
- A. Moustaj Github repo for the paper (2025).
- Y. Núñez Fernández et al., SciPost Phys. **18**, 104 (2025).
- X. Waintal et al., arXiv 2601.03035 (2026).