Tensor-Network methods for Spectral Functions of Tight-Binding models

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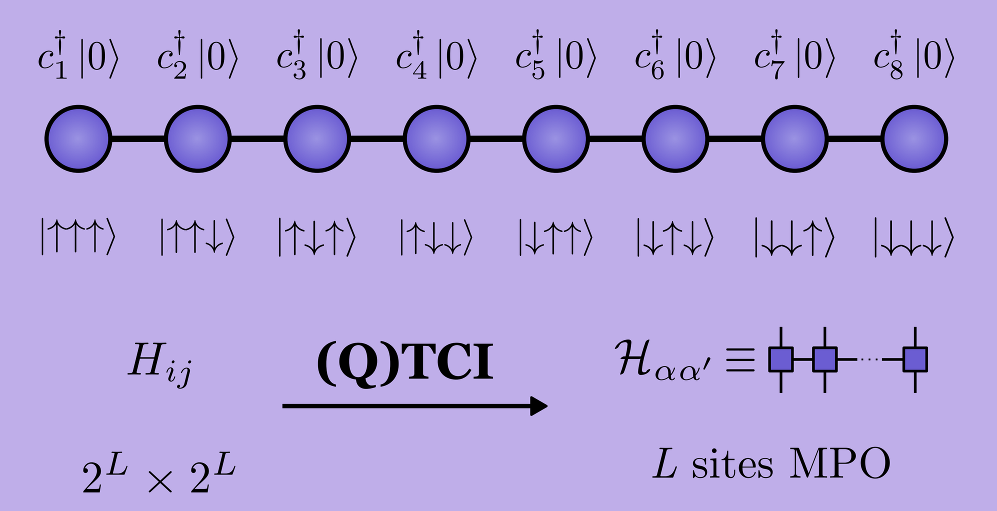
1. Introduction

We provide a new method to compute **momentum-resolved spectral functions** in moiré materials using a tensor-network formulation of **tight-binding Hamiltonians.** With (Quantics) Tensor Cross Interpolation (**QTCI**), we are able to simulate incommensurate superstructures that require **very large lattices**. Unfolded band structures can be computed, providing an essential step towards the study of **ARPES** spectra.

2. Methods

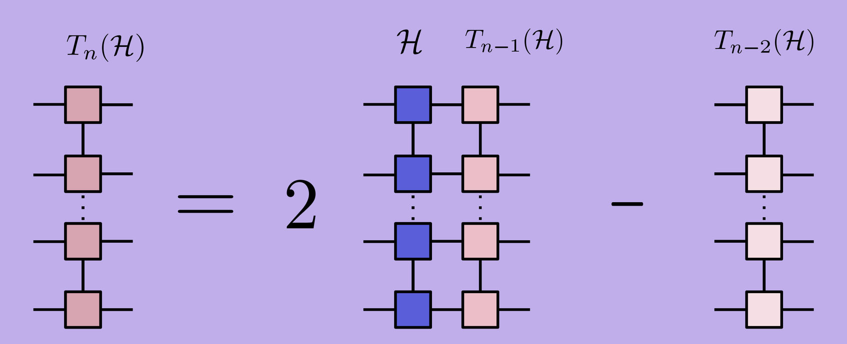
$$\hat{H} = \sum_{ij,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_{i,\sigma} V_i c^\dagger_{i\sigma} c_{i\sigma} + \sum_i U_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$

Tensor Network Representation

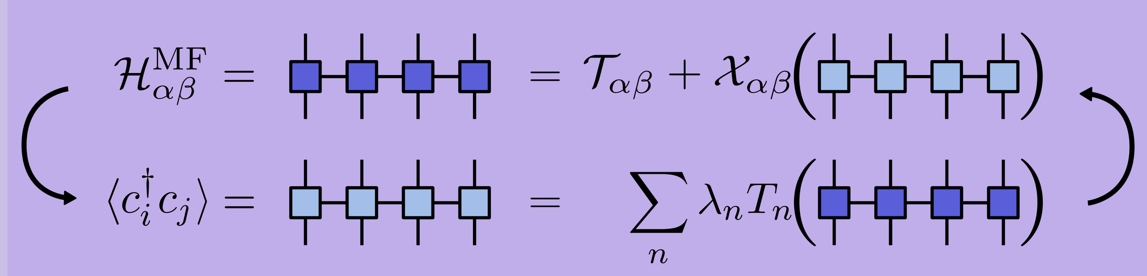


Kernel Polynomial Method

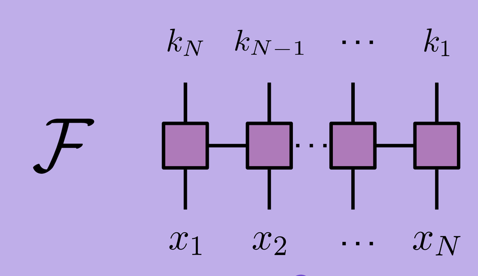
$$\delta(\omega - \hat{\mathcal{H}}) \approx \frac{1}{\pi\sqrt{1-\omega^2}} \left[\hat{I} + 2\sum_{n=1}^{N} T_n(\hat{\mathcal{H}}) T_n(\omega) \right]$$



Self-Consistent Mean Field Loop



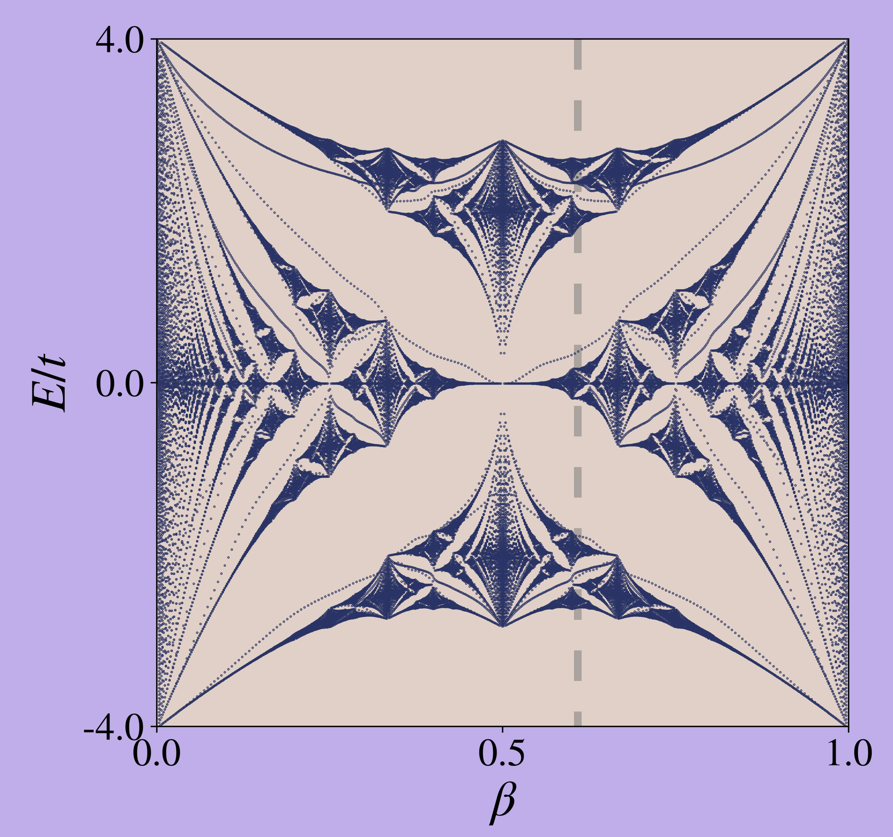
Quantum Fourier Transform



3. Results

1D: Interacting AAH Model

$$V_i = V_0 \cos\left(2\pi\beta x_i + \phi\right)$$

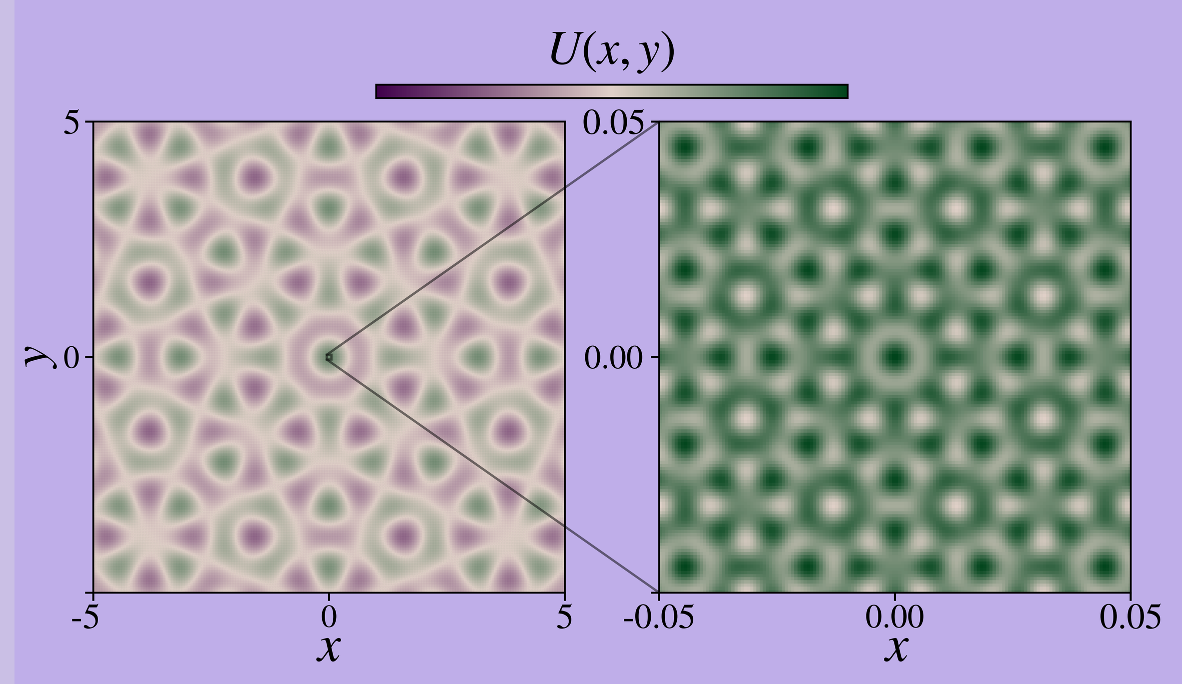


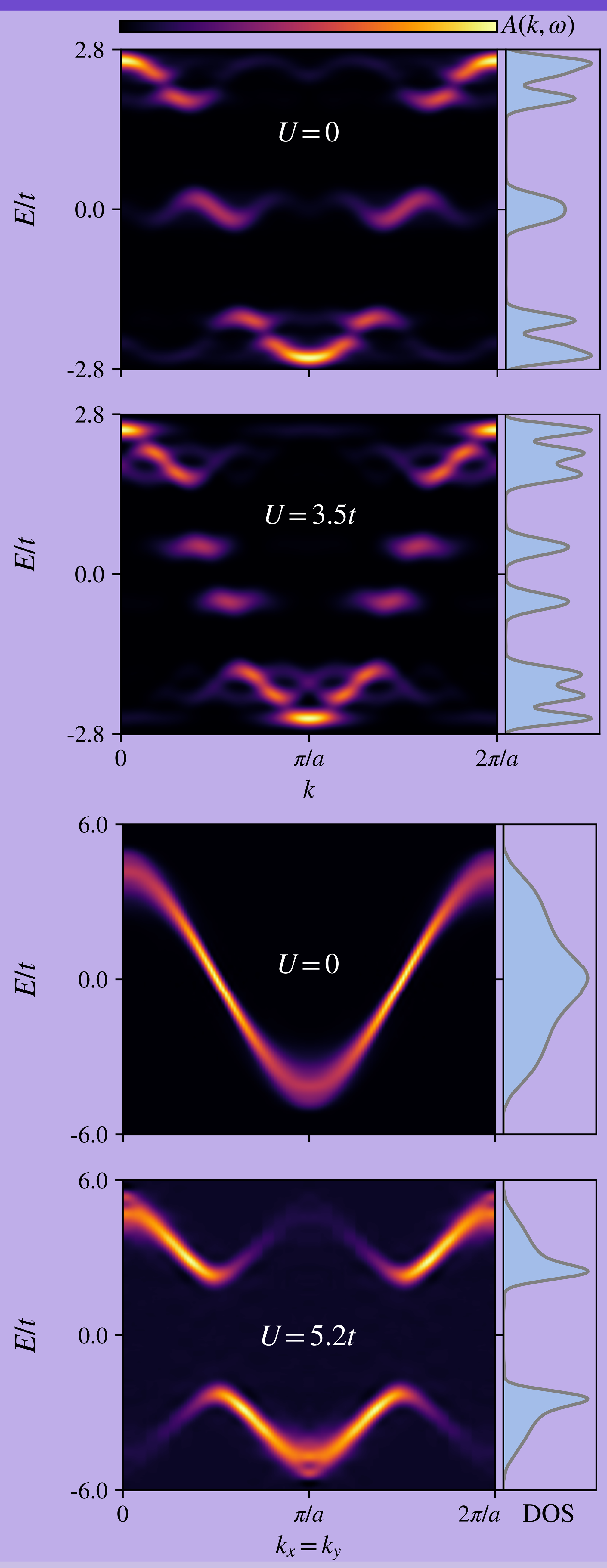
2D: Interacting 8-fold QC Model

$$U_i = U_0 \left[1 + \frac{1}{10} \sum_{n=1}^{4} \cos(\alpha \mathbf{k}_n \cdot \mathbf{x}_i) + \cos(\beta \mathbf{k}_n \cdot \mathbf{x}_i) \right]$$

Microscopic scale — Moiré scale

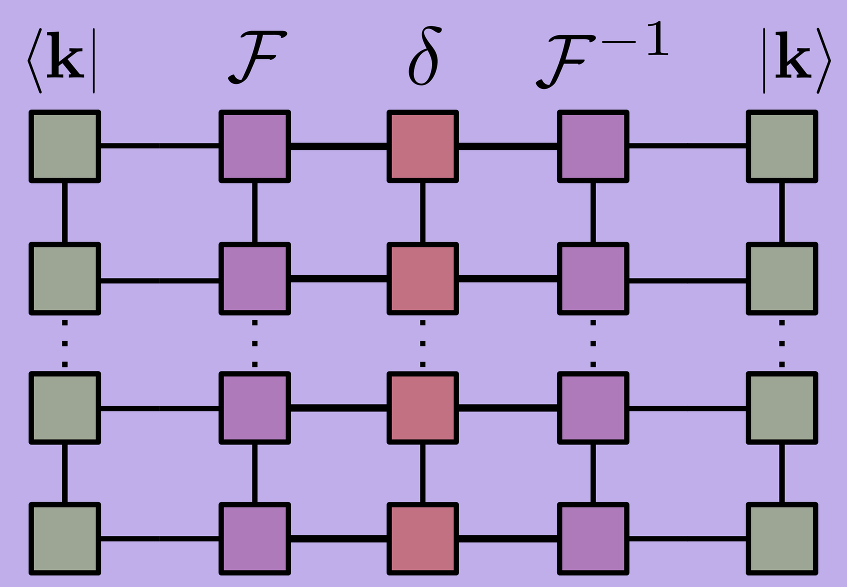
$$\mathbf{k}_n = \begin{pmatrix} \cos\left(\frac{\pi n}{4}\right) & \sin\left(\frac{\pi n}{4}\right) \\ -\sin\left(\frac{\pi n}{4}\right) & \cos\left(\frac{\pi n}{4}\right) \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$





Momentum-Resolved Spectral Function

$$A(\mathbf{k}, \omega)$$



4. Conclusion

- We use a tensor-network formalism of tight-binding models and use the **TNKPM** to compute mean-fields and spectral functions
- The **(Q)TCI** tools help speed up the calculations substantially and are perfectly suitable to use with **super moiré modulations**
- By using the QFT, we can compute the **momentum-resolved spectral function**, an essential tool to study **ARPES** spectra
- **Outlook**: Apply to realistic models

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References:
- ArXiv 2503.04373
- ArXiv 2506.05230
- This work will soon appear on arXiv