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

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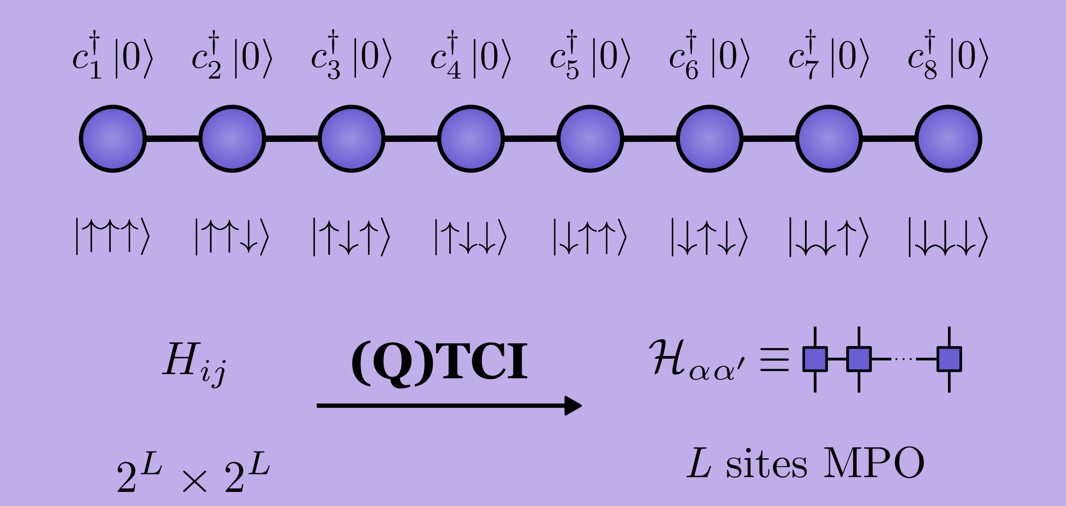
1. Introduction

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 tool for simulating **ARPES** or **QTM** data

2. Methods

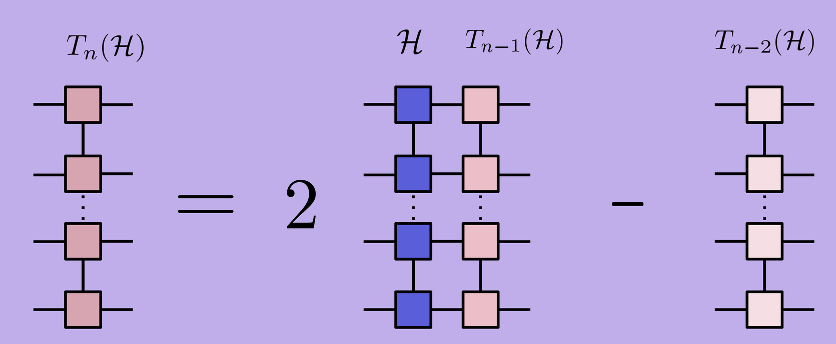
$$\hat{H} = \sum_{ij,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_{i,\sigma} V_i c^\dagger_{i\sigma} c_{i\sigma} + \sum_i U_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$

Tensor Network Representation

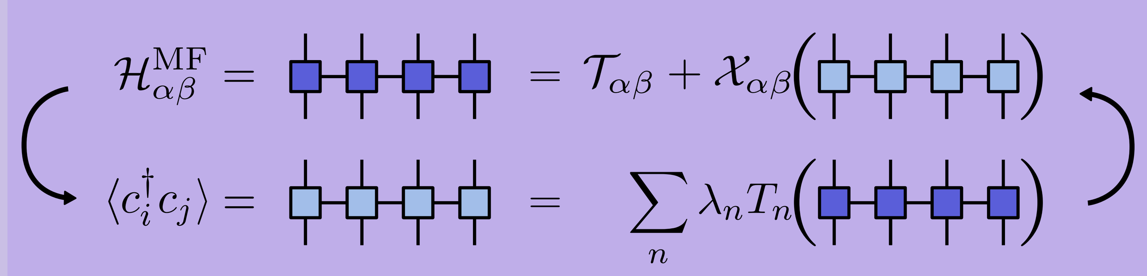


Kernel Polynomial Method

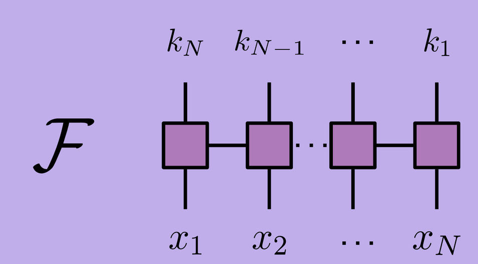
$$\delta(\omega - \hat{\mathcal{H}}) \approx \frac{1}{\pi\sqrt{1-\omega^2}} \left[\hat{I} + 2\sum_{n=1}^{N} T_n(\hat{\mathcal{H}}) T_n(\omega) \right]$$



Self-Consistent Mean Field Loop

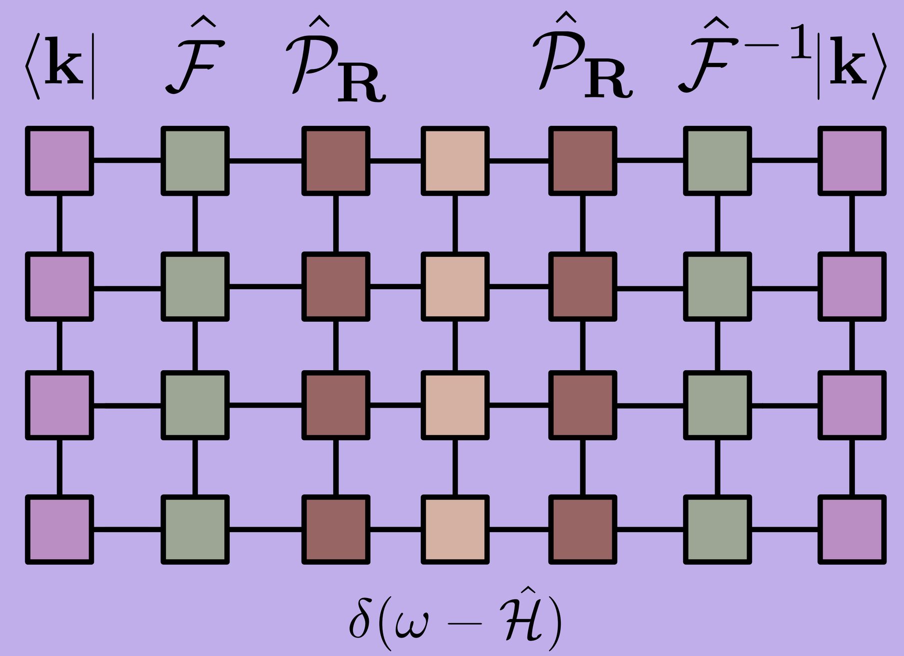


Quantum Fourier Transform



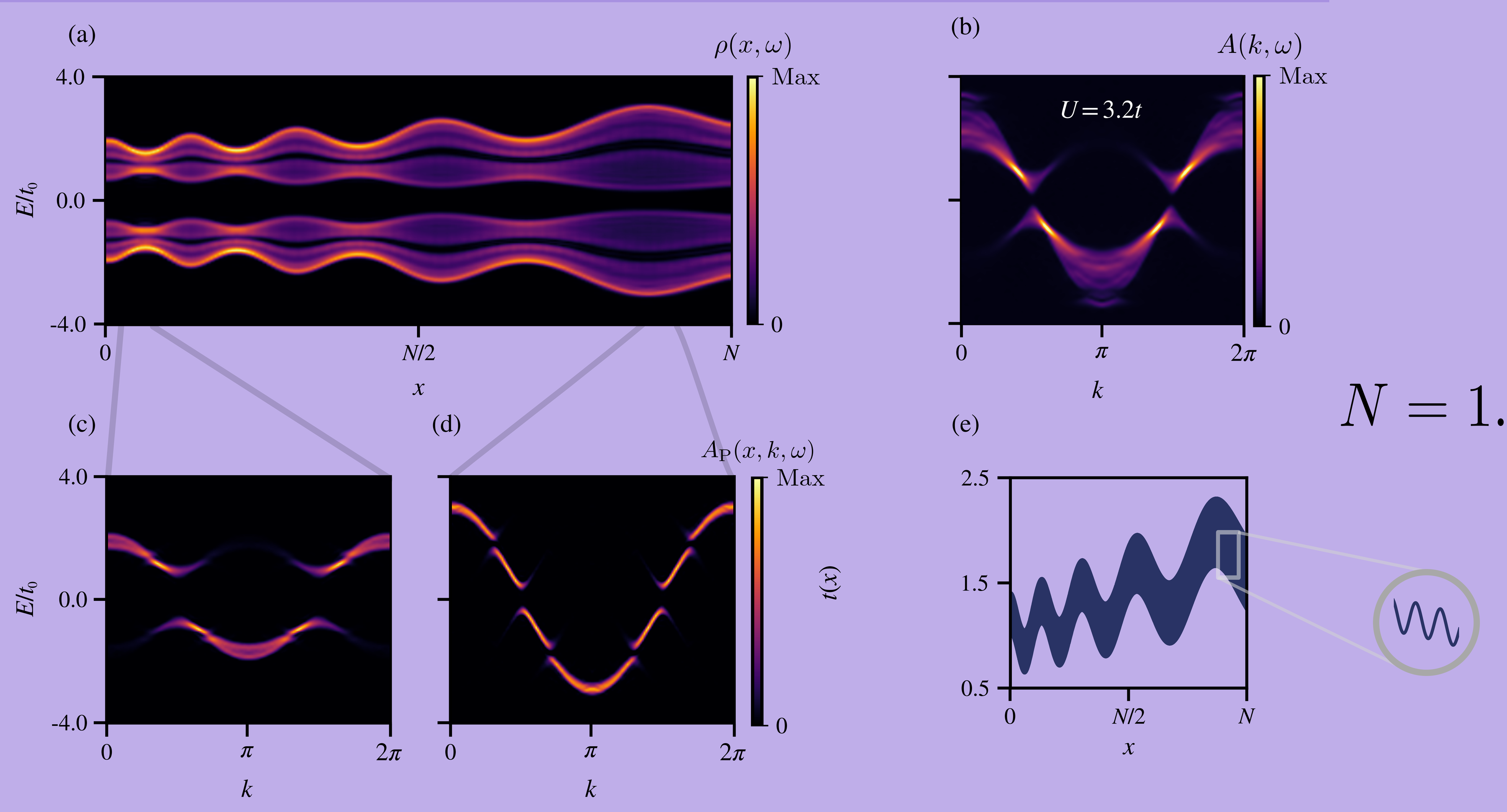
Local Momentum-Resolved Spectral Function

$$A_{\mathrm{P}}(\mathbf{R}, \mathbf{k}, \omega)$$



3. Results

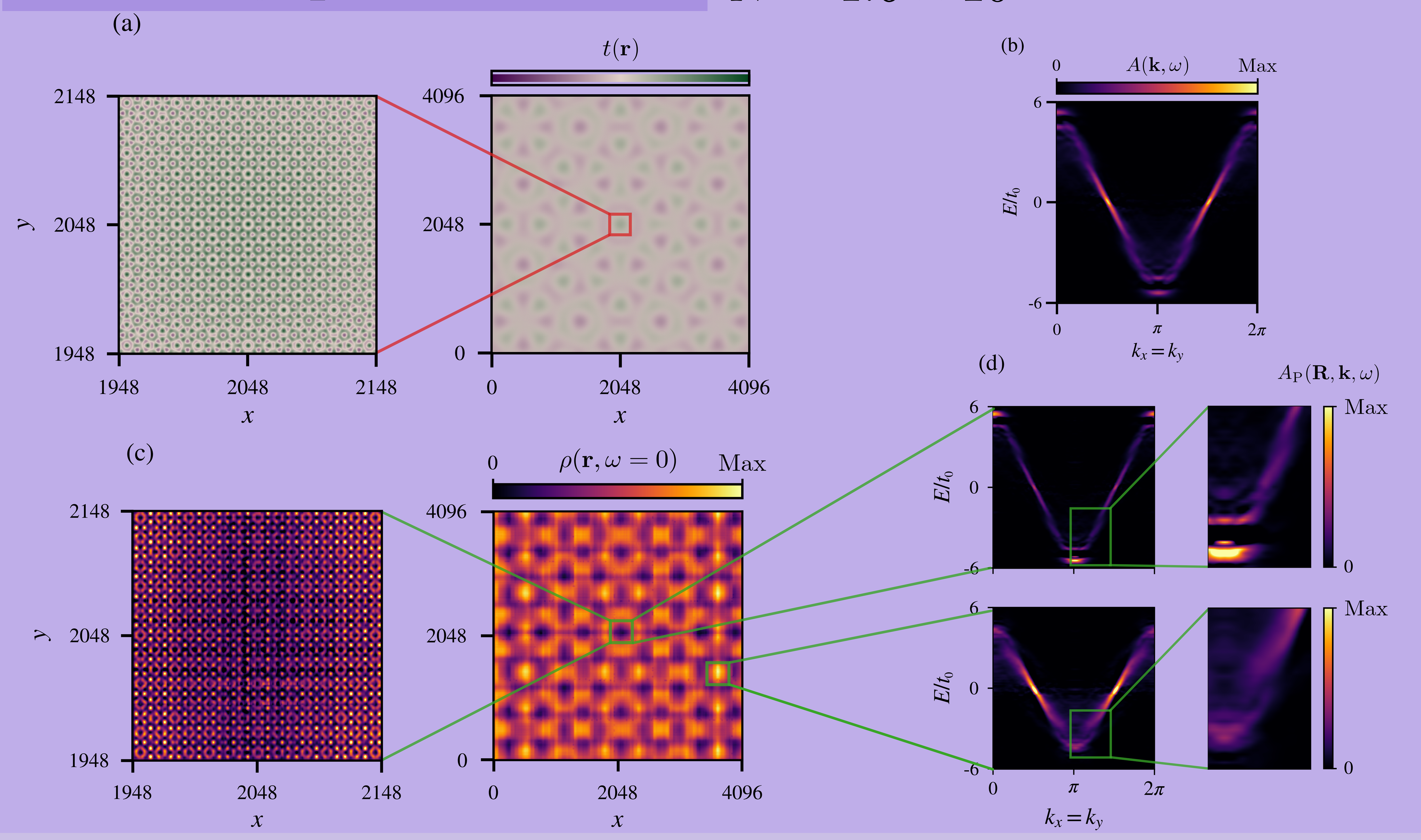
1D: Interacting chain with inhomogeneous strain



$N = 1.6 \times 10^7$

2D: 8-fold QP potential

$N = 1.6 \times 10^7$



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 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
- We can also resolve momentum dependence locally in space, like the **Quantum Twisting Microscope**

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References:
- ArXiv 2503.04373
- ArXiv 2506.05230
- ArXiv 2512.18397