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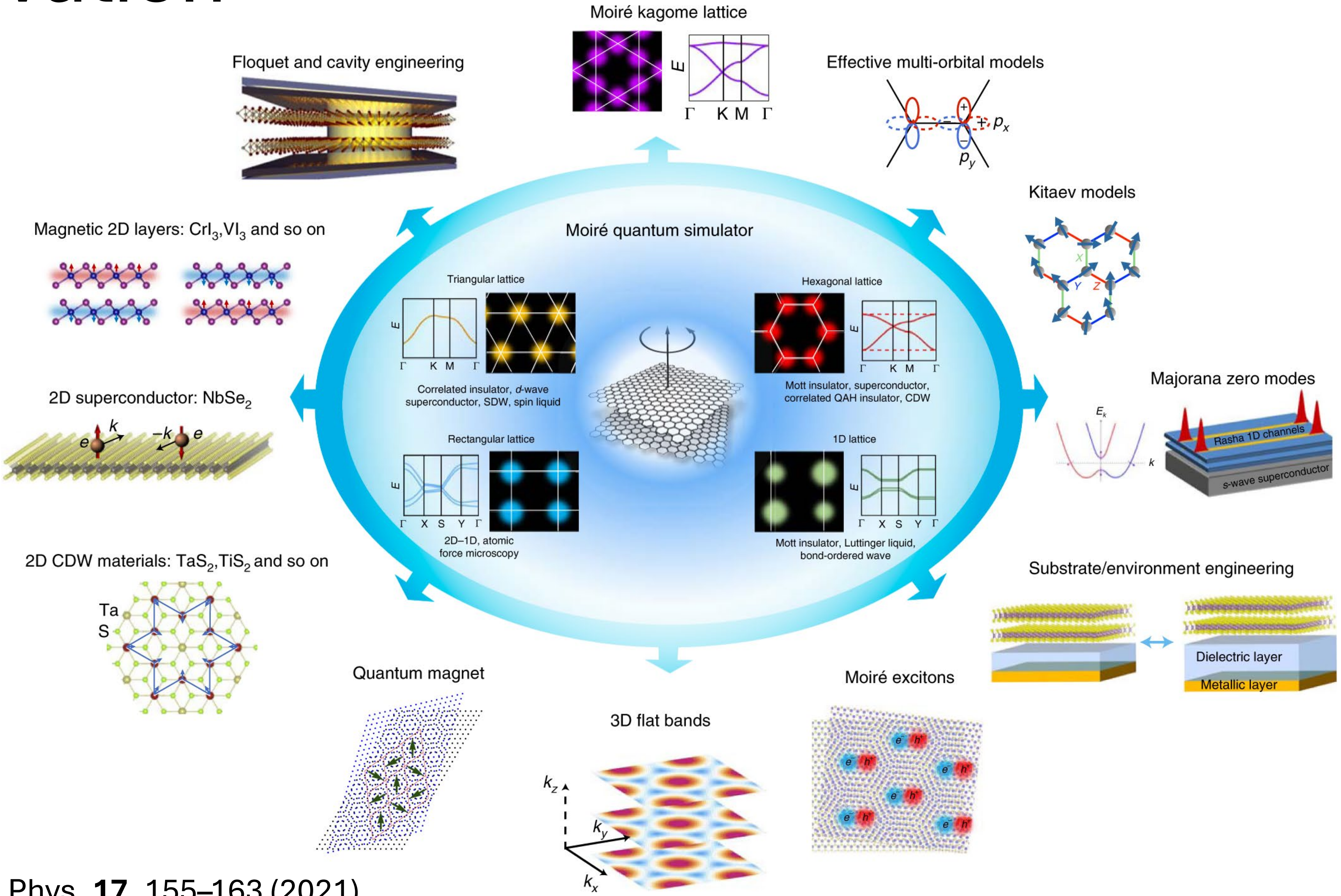
arXiv 2512.18397 (2025)

Tensor network approach to momentum-resolved spectroscopy in non-periodic super-moiré systems

Anouar Moustaj, Yitao Sun, Tiago Antão, Jose Lado

Motivation



Kennes et al. – Nat. Phys. **17**, 155–163 (2021)

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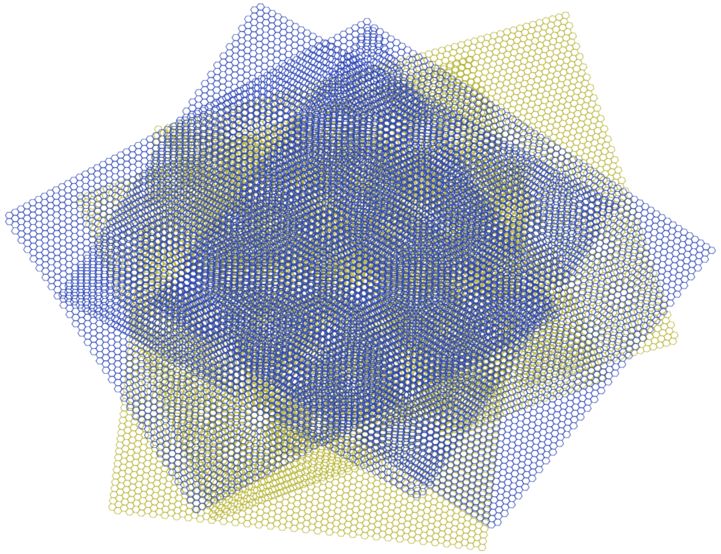
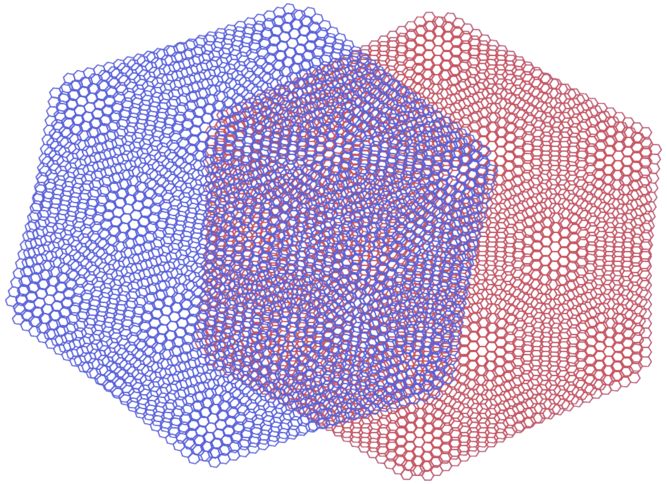
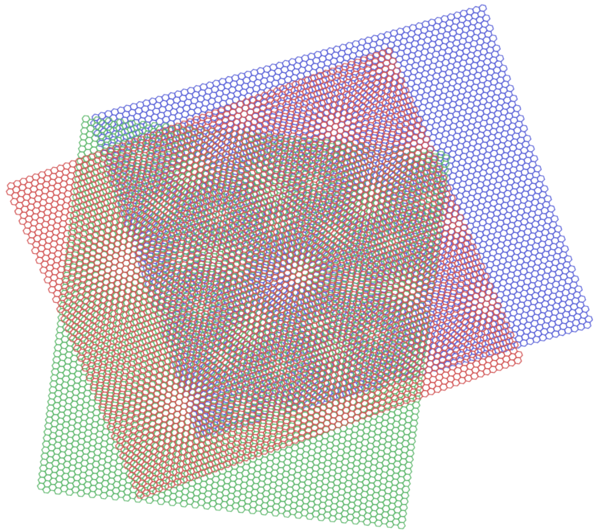
Motivation – Limitations





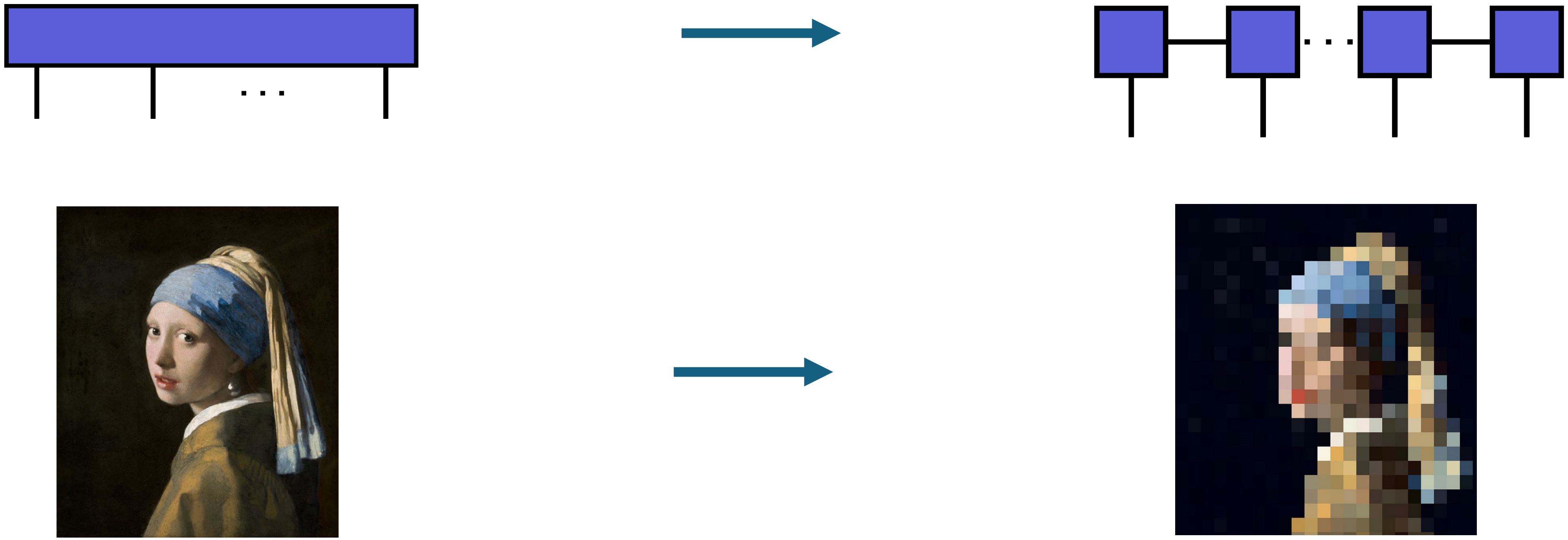


Sizes $\gtrsim 10^9$ →

- Storage issues: not enough RAM
- Computation times: days to years

Quantum many-body physics

- Decades of dealing with exponentially large Hilbert space
- Tensor-network schemes are now very powerful



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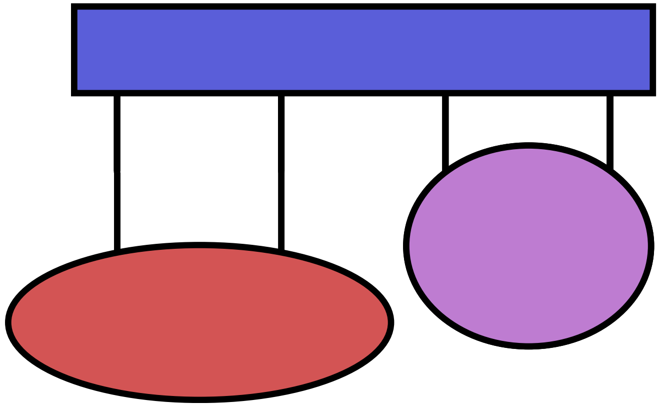
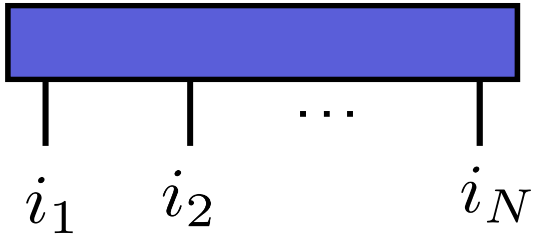
Tensor-Networks Crash Course

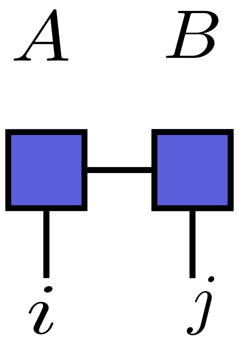


Tensor Network

$C_{i_1 i_2 \cdots i_N}$



$$C_{ij} = \sum_k A_{ik} B_{kj} =$$



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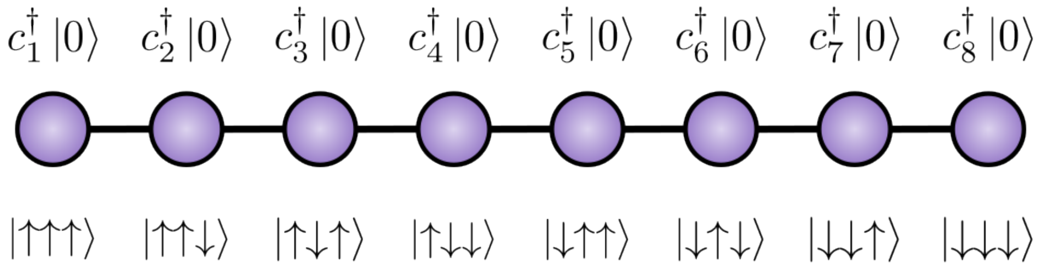
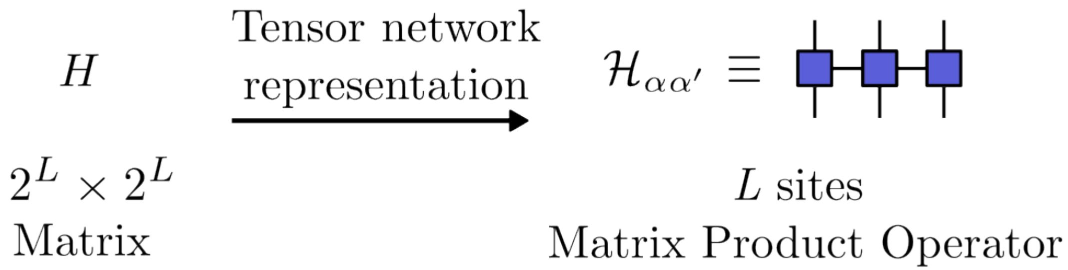
Tight-Binding Hamiltonians as MPOs

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





Density of states

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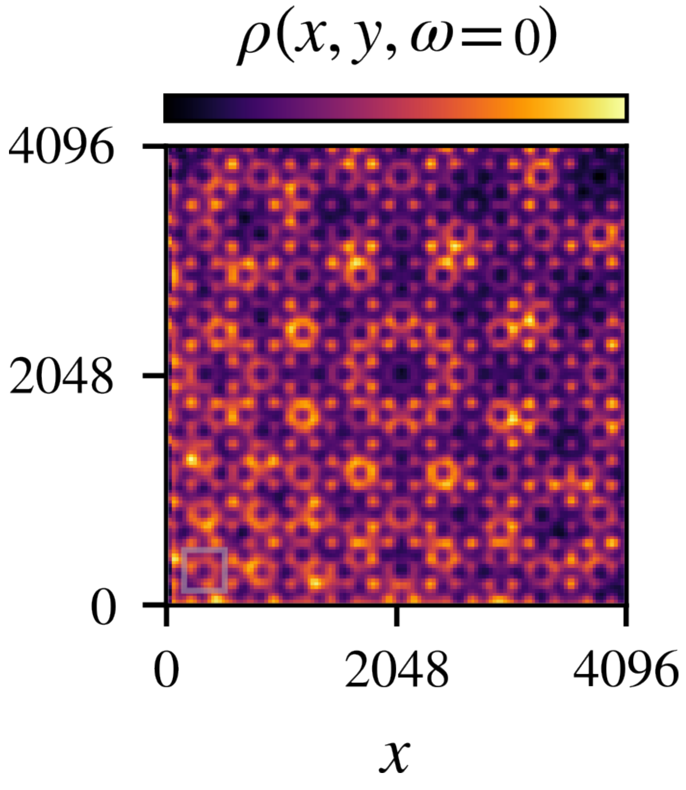
$$\rho(\mathbf{x}, \omega) = \langle \mathbf{x} | \, \delta(\omega - \hat{\mathcal{H}}) \, | \mathbf{x} \rangle$$

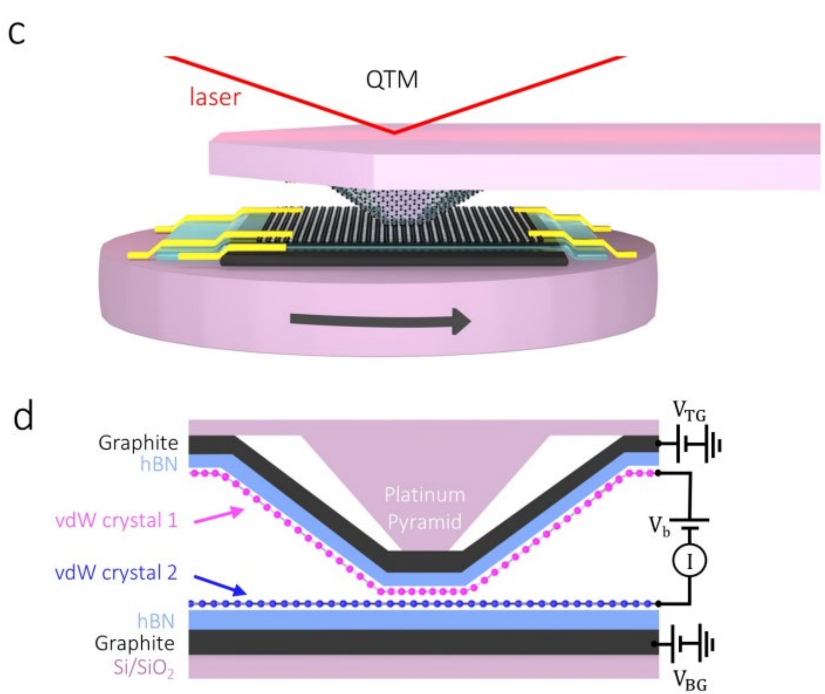
LDOS

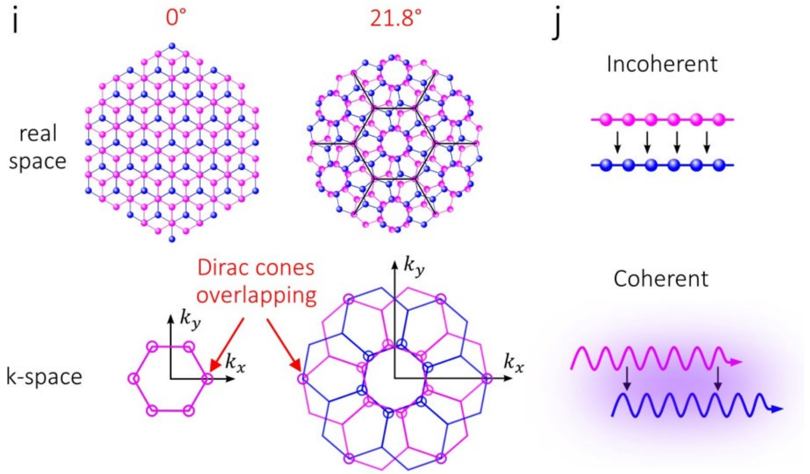
$$\delta(\omega - \hat{\mathcal{H}}) \approx \frac{1}{\pi\sqrt{1-\omega^2}} \left[\hat{1} + 2 \sum_{n=1}^{N} T_n(\hat{\mathcal{H}}) T_n(\omega) \right]$$

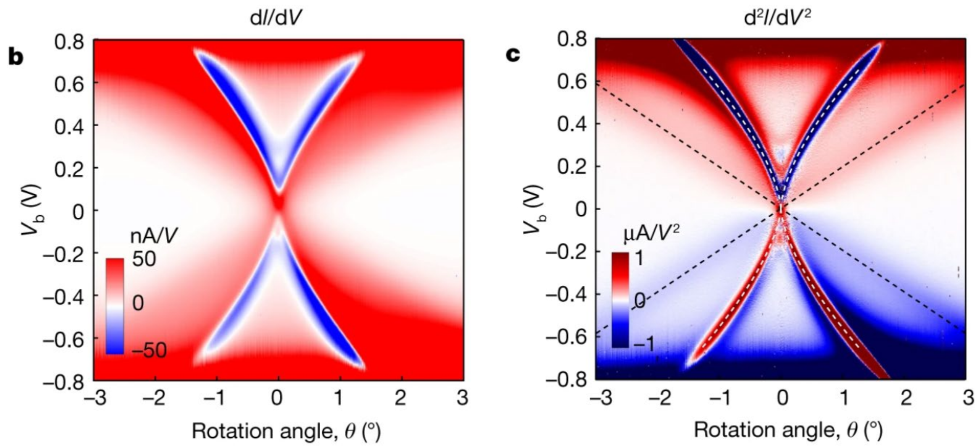
$$T_0(x) = 1, \quad T_1(x) = x, \quad T_n(x) = 2x T_{n-1}(x) - T_{n-2}(x)$$



Probing momentum space locally







A. Inbar et al. – Nature **614**, 682–687 (2023)

Probing momentum space locally

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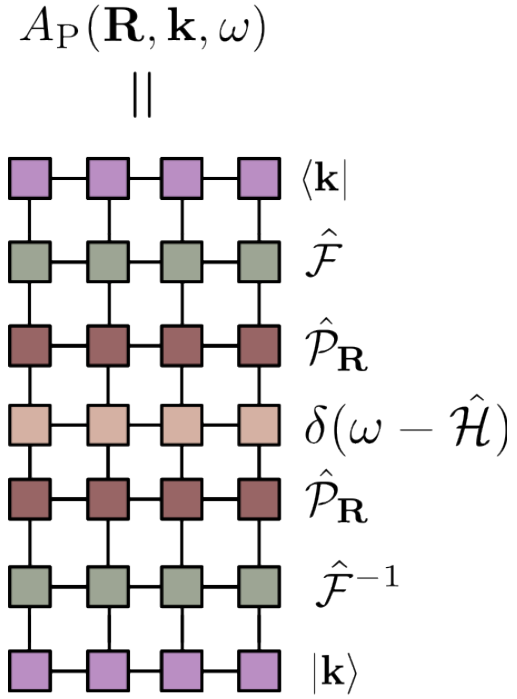
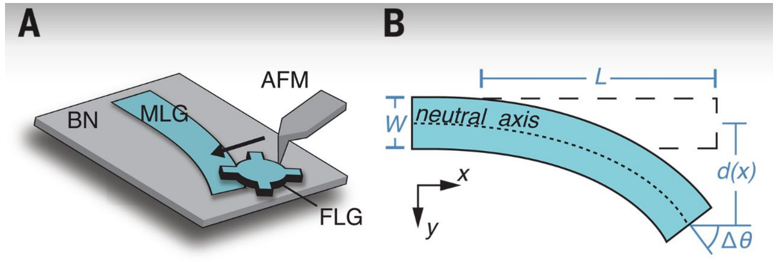
$$\mathcal{A}(\mathbf{k},\omega) = \langle \mathbf{k}| \hat{\mathcal{F}} \delta(\omega - \hat{\mathcal{H}}) \hat{\mathcal{F}}^{-1} |\mathbf{k}\rangle$$

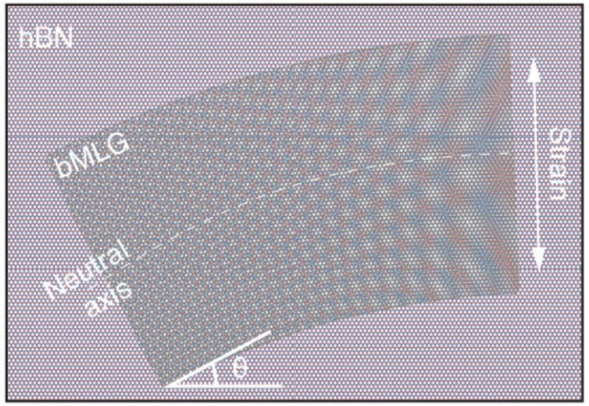
⬇

$$A_{\mathrm{P}}(\mathbf{R},\mathbf{k},\omega) = \langle \mathbf{k}| \hat{\mathcal{F}} \hat{\mathcal{P}}_{\mathbf{R}} \delta\left(\omega - \hat{\mathcal{H}}\right) \hat{\mathcal{P}}_{\mathbf{R}} \hat{\mathcal{F}}^{-1} |\mathbf{k}\rangle$$

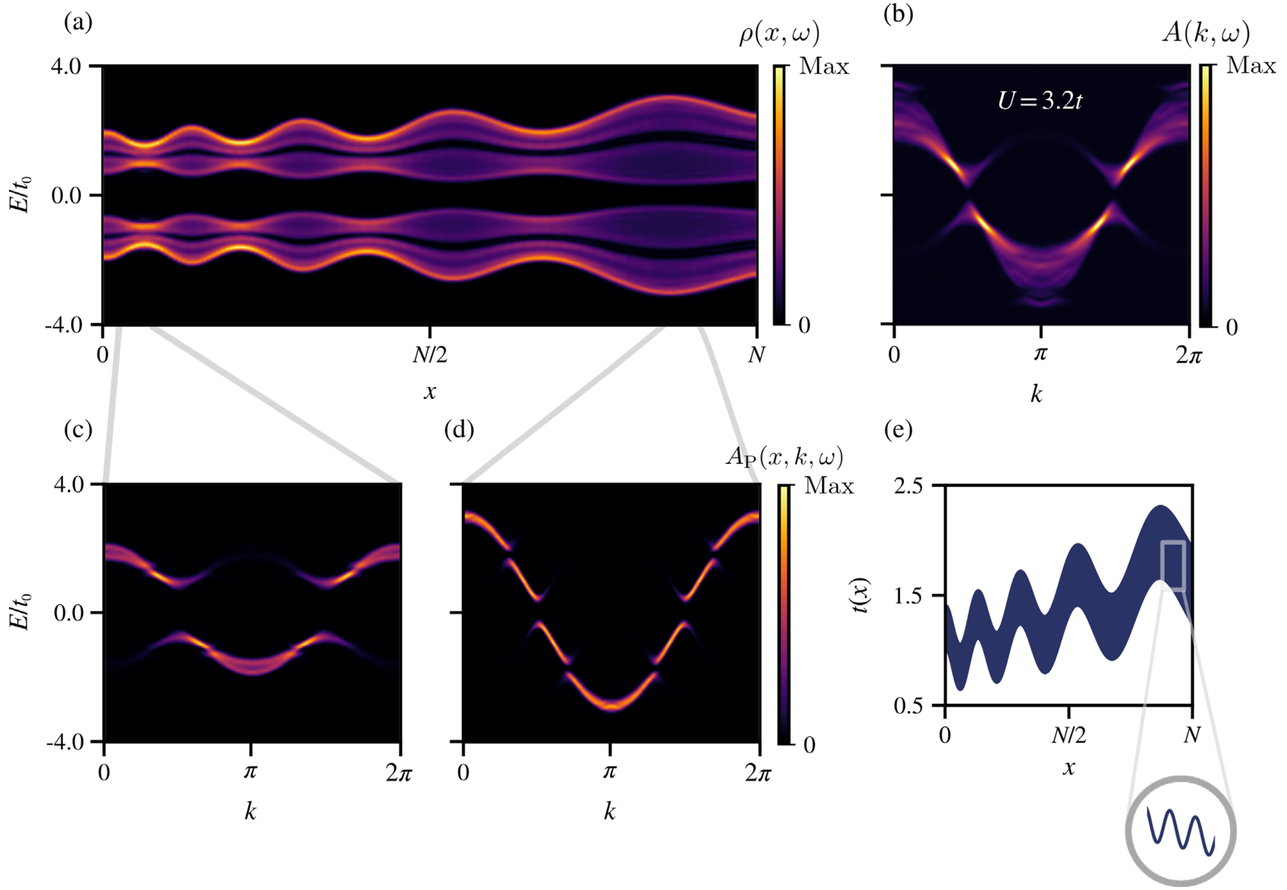


1D: Interacting chain with inhomogeneous strain





$$N = 1.6 \times 10^7$$

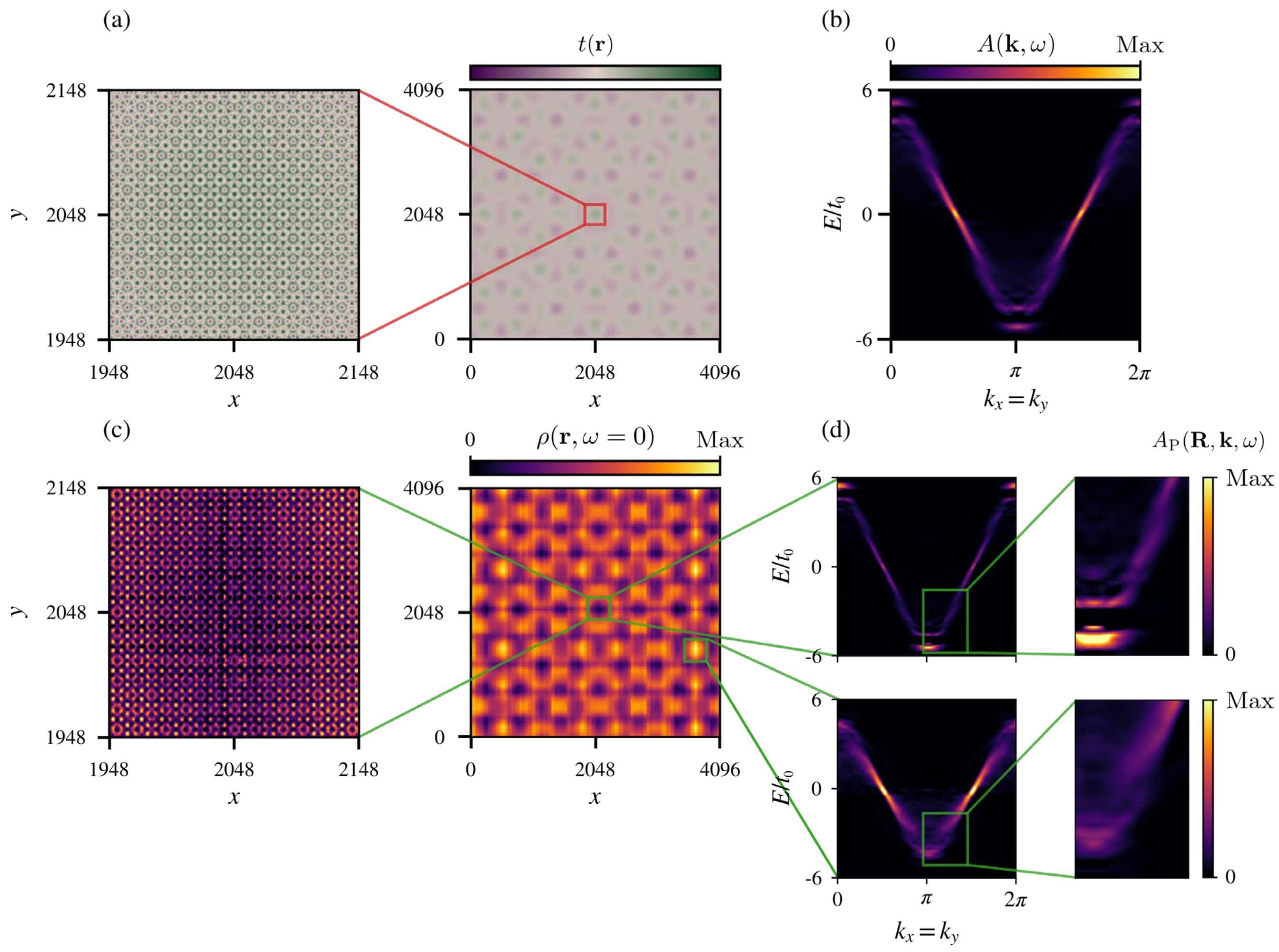


M. Kapfer et al. – Science **381**, 6658, 677-681 (2023)

A. Moustaj et al. – arXiv 2512.18397 (2025)

2D: Quasiperiodic super-moiré potential

$$N = 1.6 \times 10^7$$



A. Moustaj et al. – arXiv 2512.18397 (2025)

Take-home message

- Tight-binding simulations up to million–billion site systems
- Method based on tensor-network compression
- Quantum Fourier Transform implemented as MPO
- Direct access to local momentum-resolved spectral functions
- Applicable to moiré / super-moiré systems
- Provides a simulation tool for ARPES/QTM

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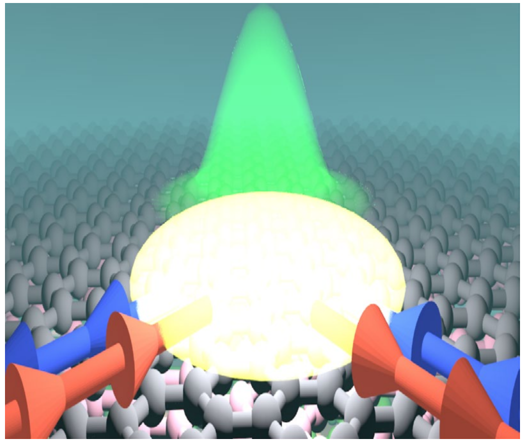
Tiago Antão



CQM group