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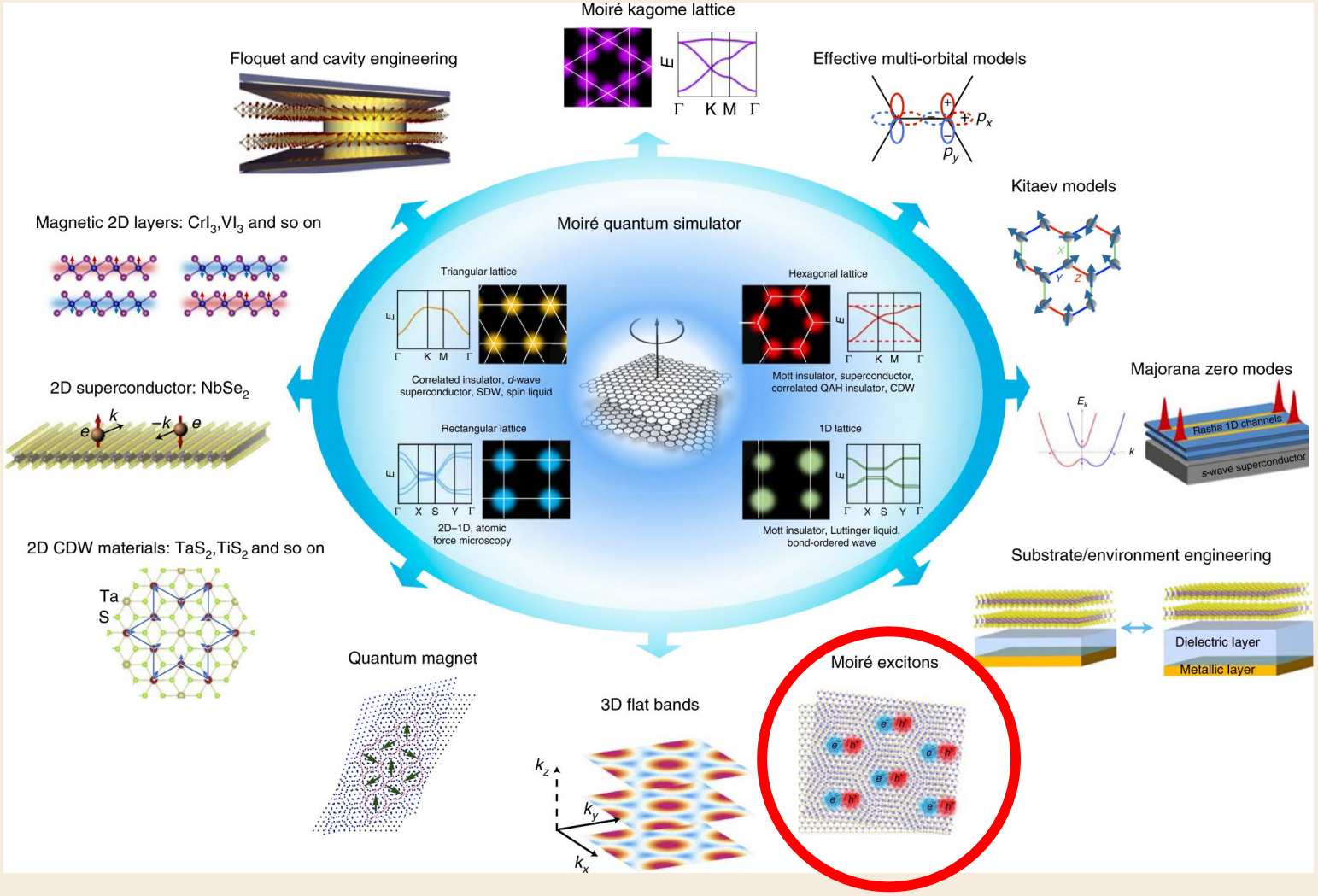
Tensor-network methodology for real-space super-moiré excitons

Anouar Moustaj, Yitao Sun, Tiago Antão, Lumen Eek, Jose Lado

ArXiv 2607.00991

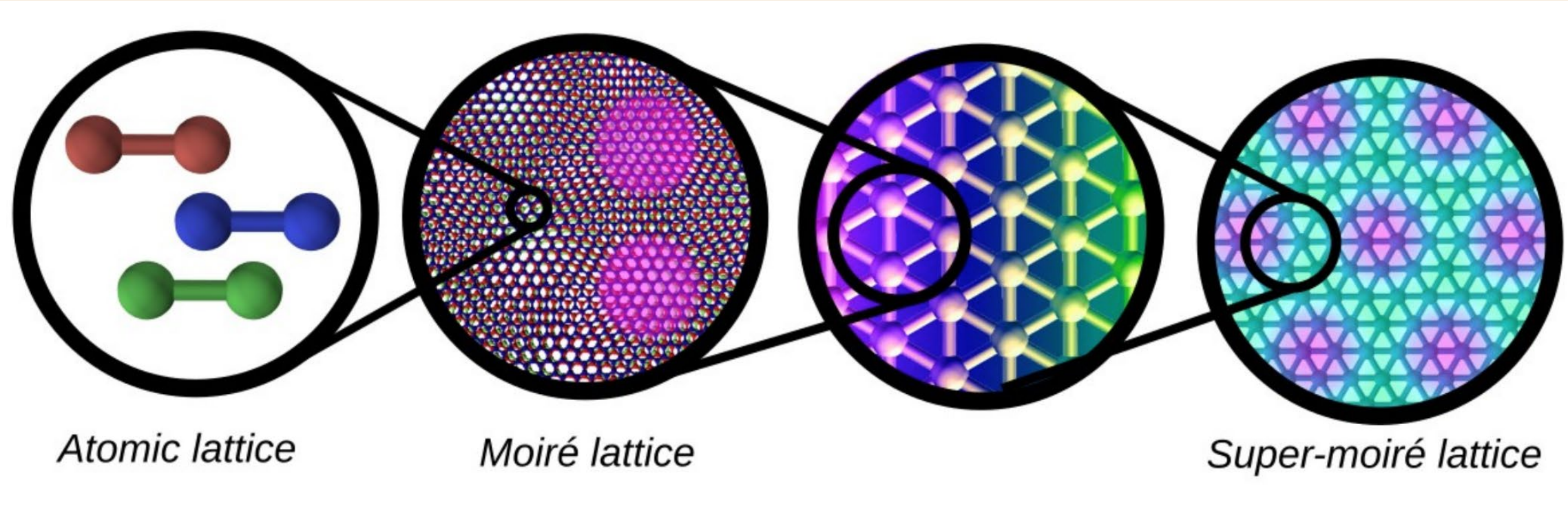
ArXiv 2603.02011

Motivation



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

Motivation

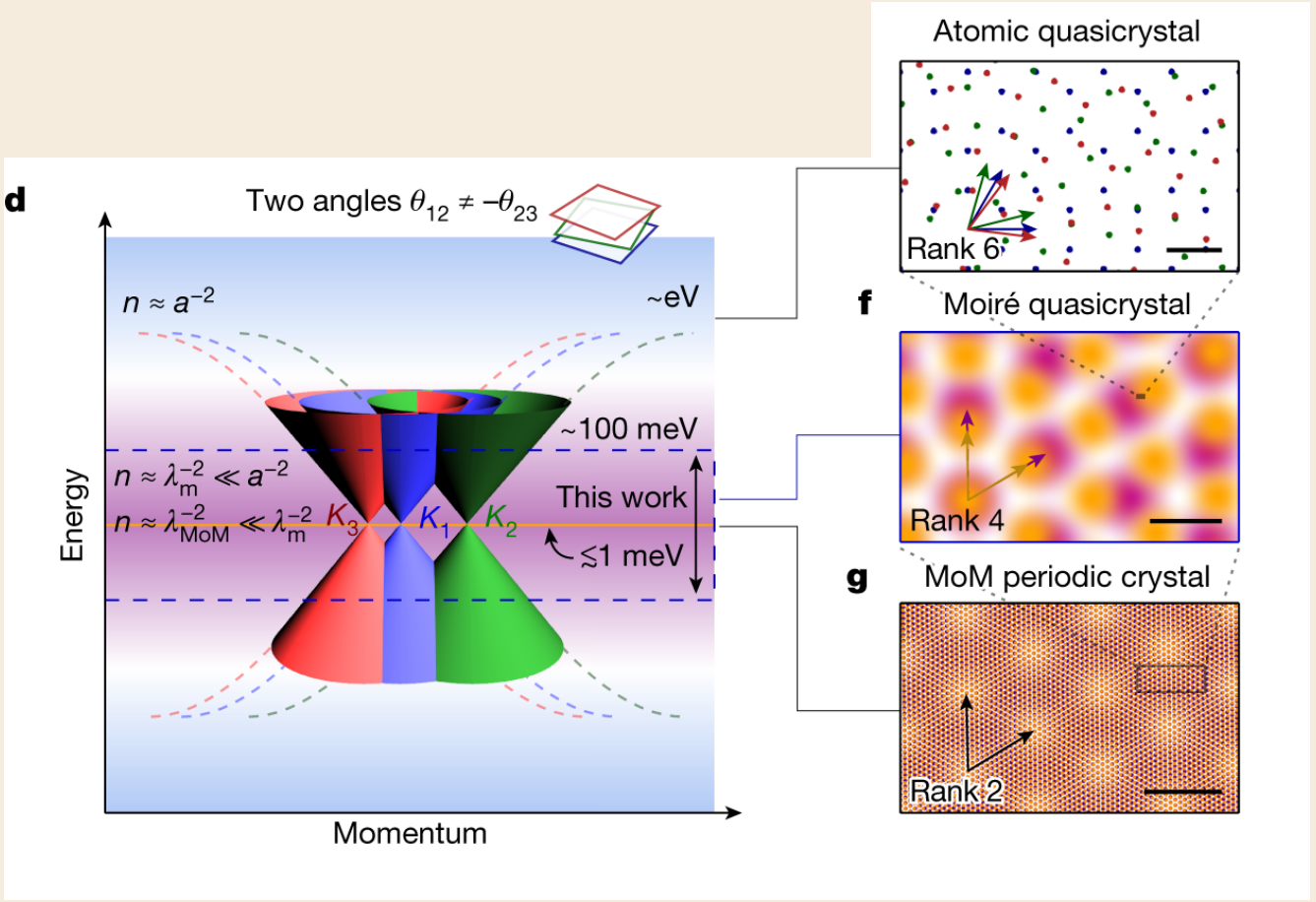


A. Uri et al., Nature 620, 762-767 (2023)

C. Y. Hao et al., Nat. Commun. 15, 8473 (2024)

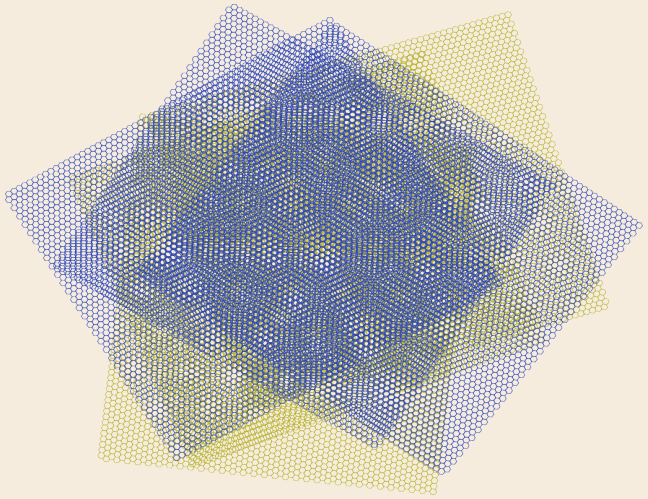
D. Park et al., Nature 641, 896–903 (2025)

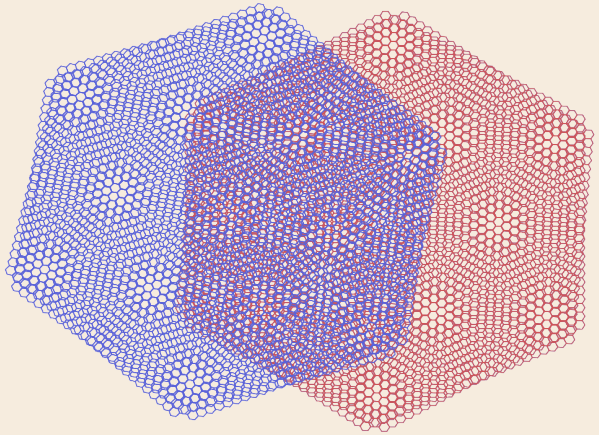
Motivation

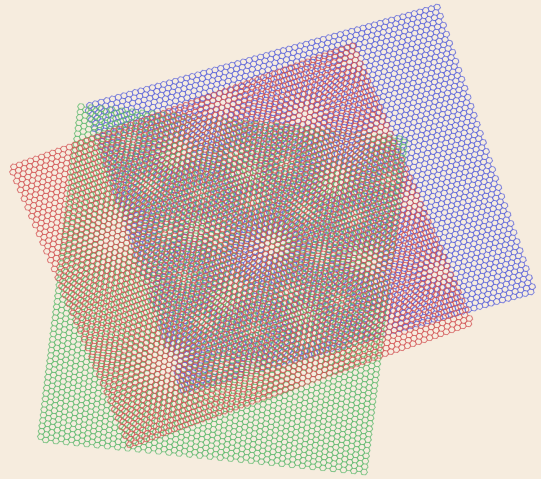


A. Uri et al., Nature 620, 762-767 (2023)

Motivation







SIZE

$$\gtrsim 10^9$$

BSE HAMILTONIAN

$$\gtrsim 10^{18} \times 10^{18}$$

O(N^4)

ISSUES

- Storage
- Computation times

Content

Aalto University
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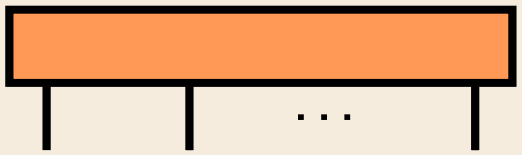
1. Motivation
2. Tensor Networks
3. Tight-Binding in the Tensor Network Formulation
4. Tensor-Network representation of the BSE
5. Spectral function: Tensor-Network KPM
6. Application to simple models
7. Conclusion and outlook

Tensor Networks

- Many-body numerical methods: decades of dealing with exponentially large objects
- Tensor-network algorithms are well-developed: good compression schemes

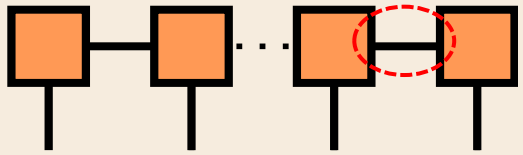
$$|\psi\rangle = \sum_{\sigma_1\sigma_2\cdots\sigma_L} \psi_{\sigma_1\sigma_2\cdots\sigma_L} |\sigma_1\sigma_2\cdots\sigma_L\rangle$$

d^L elements



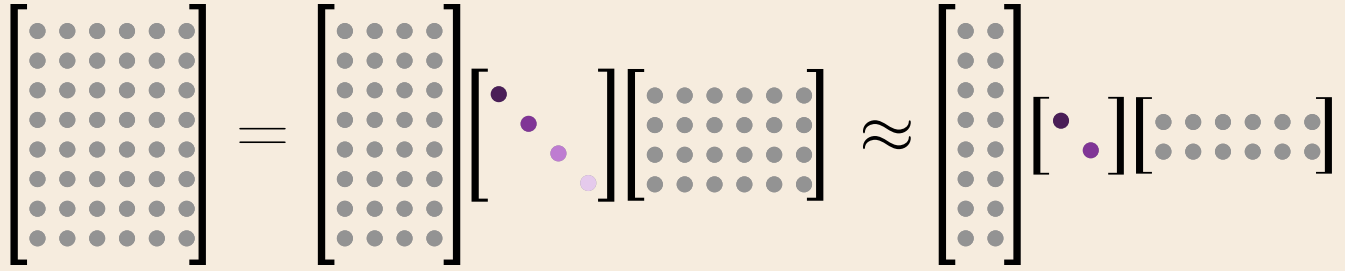
$$|\psi\rangle = \sum_{\sigma_1\sigma_2\cdots\sigma_L} M^{(1)}_{\sigma_1} M^{(2)}_{\sigma_2} \cdots M^{(L)}_{\sigma_L} |\sigma_1\sigma_2\cdots\sigma_L\rangle$$

$L\chi^2$ elements



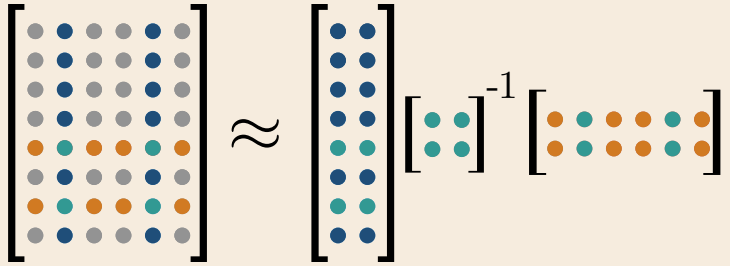
Compression schemes

- SVD



$$\epsilon_{\text{svd}} = \sum_{r+1}^{Q} \lambda_k^2$$

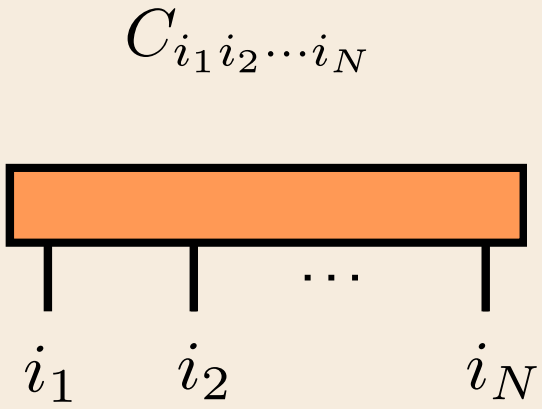
- Cross Interpolation

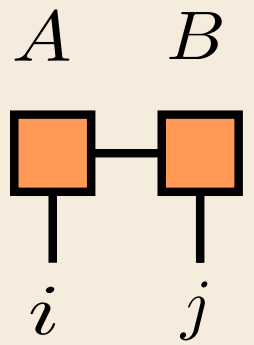


Active learning of matrix/tensor

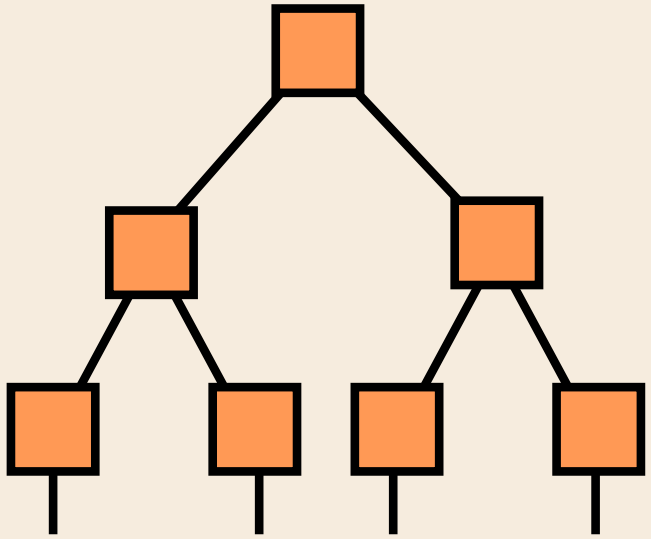
$$\epsilon_{\text{ci}} = (1+\delta)\,\epsilon_{\text{svd}}$$

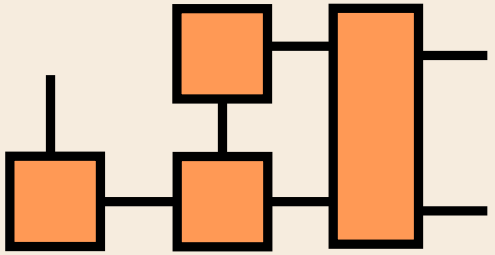
Tensor Networks

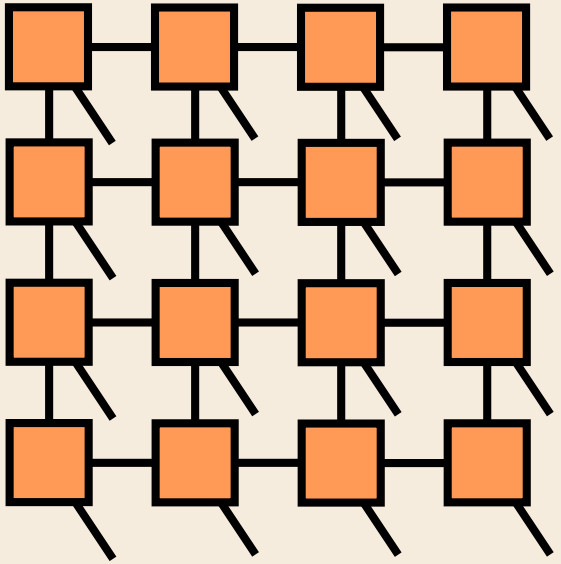




$$C_{ij} = \sum_k A_{ik} B_{kj}$$

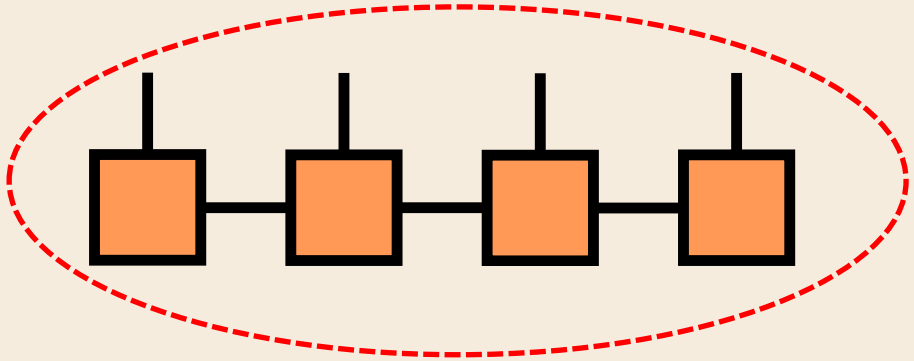


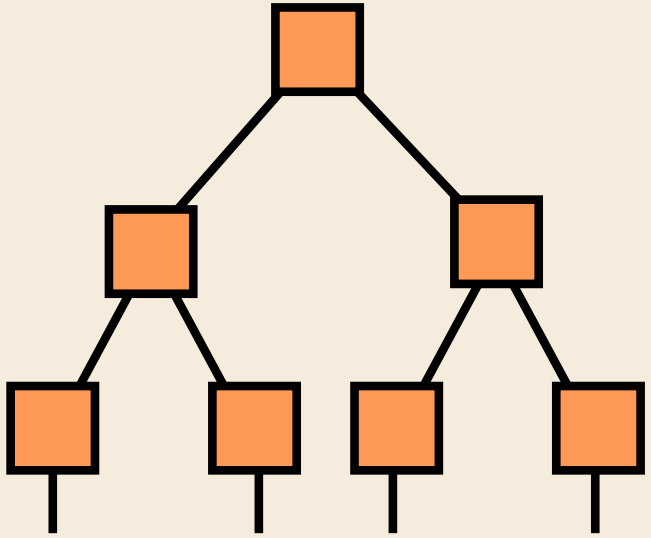


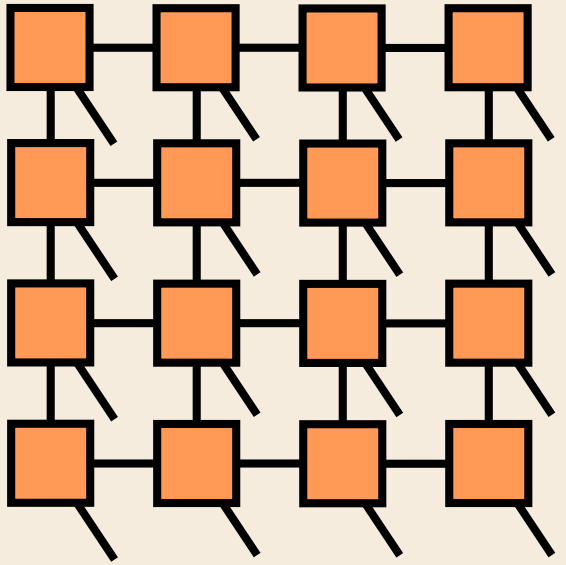


Tensor Network

Tensor Train (MPS)



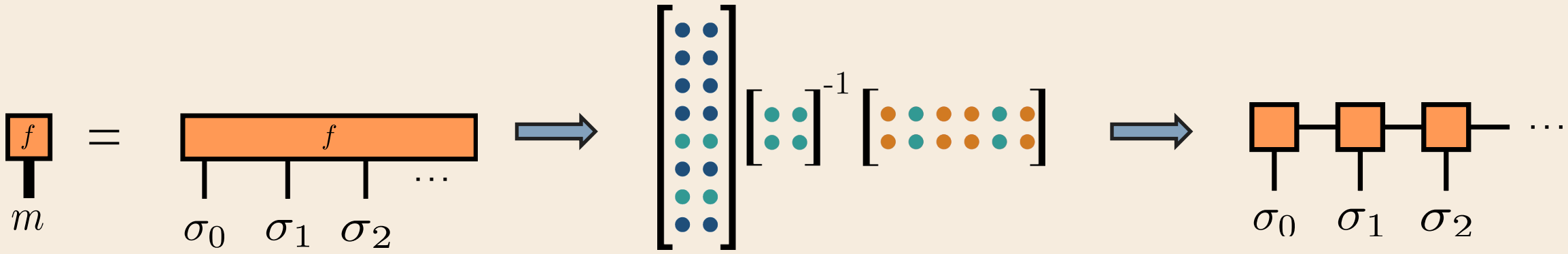




Tensor Trains – Function Approximators

$$f(x_m) \equiv f_m = f\left(m = \sum_{n=0}^{L-1} \sigma_n 2^{L-n}\right) = f_{\sigma_0 \sigma_1 \sigma_2 \cdots}$$

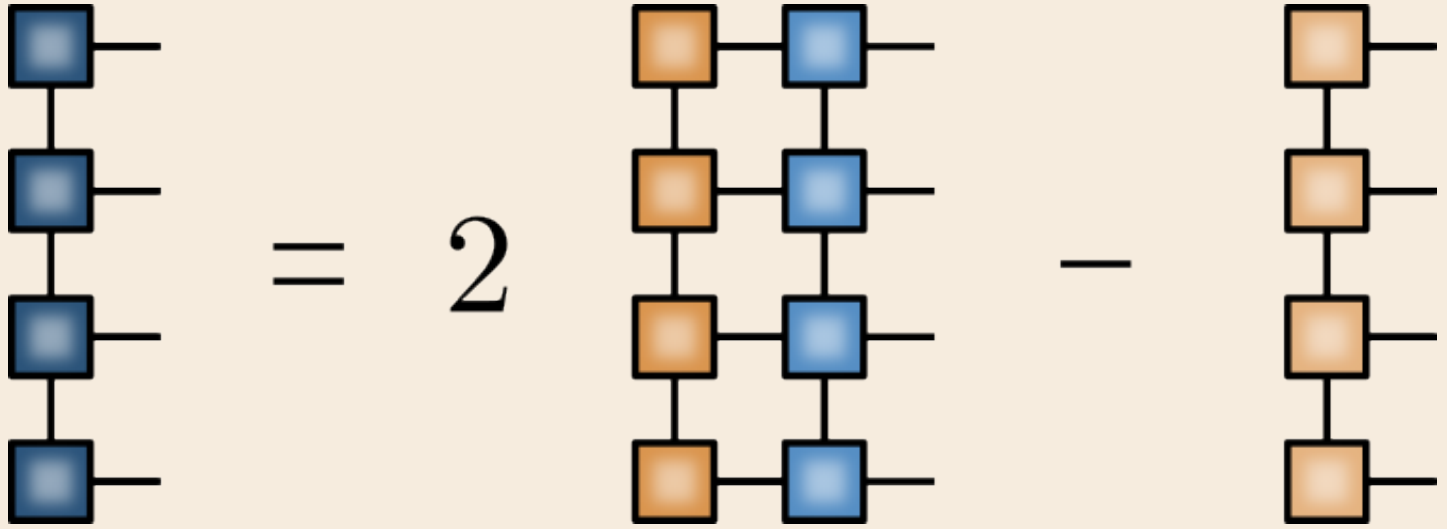
TCI



M.K Ritter, Phys. Rev. Lett. 132, 056501 (2024)

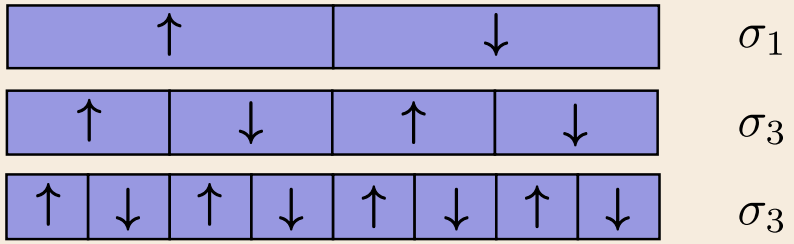
Tensor Train Algebra

$$A_{\sigma_1\sigma_2\cdots} = 2 \sum_{\sigma_1'\sigma_2'\cdots} B^{\sigma_1'\sigma_2'\cdots}_{\sigma_1\sigma_2\cdots} C_{\sigma_1'\sigma_2'\cdots} - D_{\sigma_1\sigma_2\cdots}$$

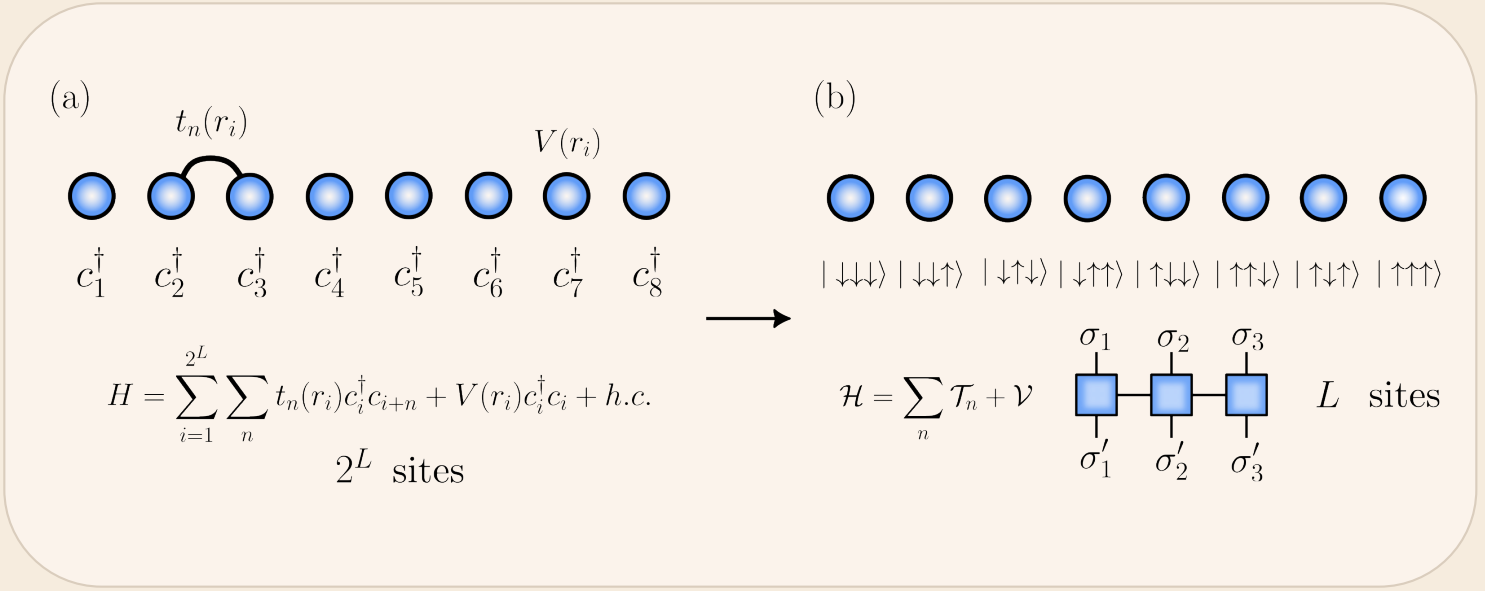


Single-Particle Tight-binding Hamiltonians

Tight-Binding Hamiltonians as Matrix Product Operators

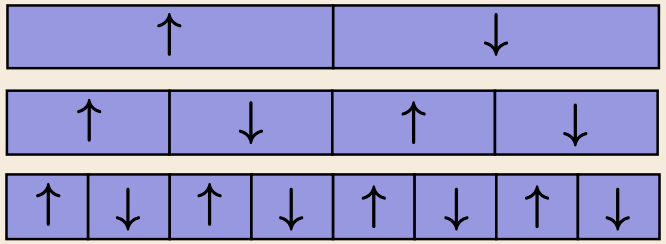


- Pseudospin basis (quantics)
- The Hamiltonian becomes an MPO on L = $\log_2$N sites.

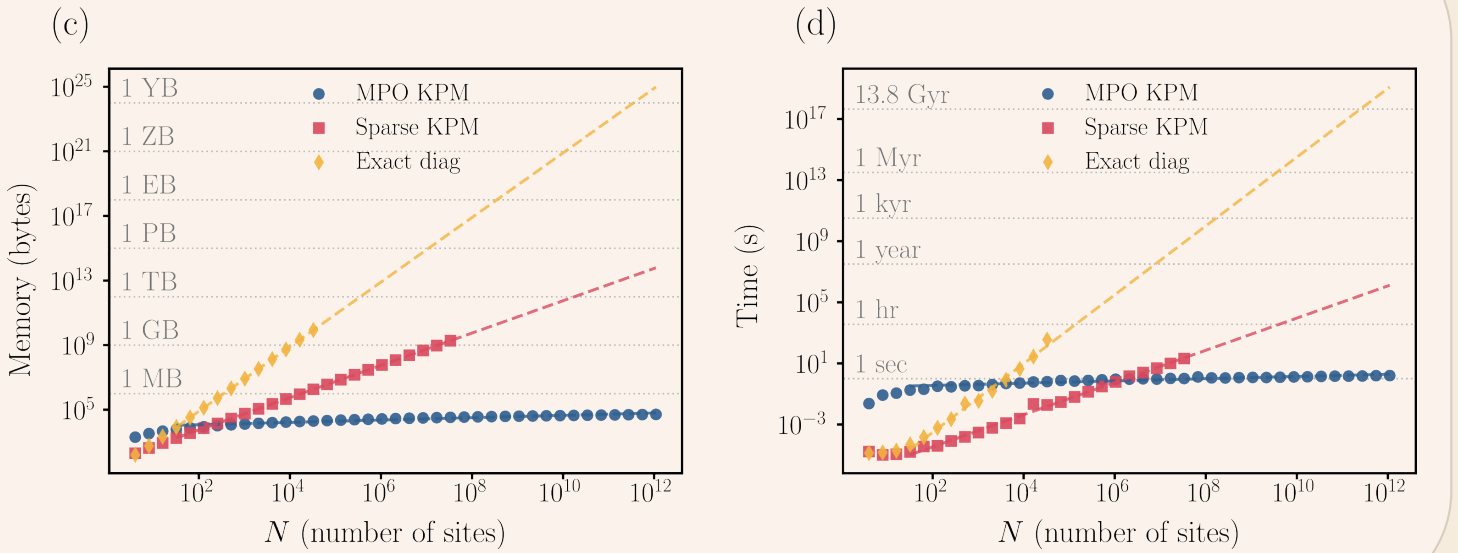


T. Antão, A. Moustaj, Y. Sun, J. Lado arXiv 2607.00991 (2026)

Tight-Binding Hamiltonians as Matrix Product Operators



- Pseudospin basis (quantics)
- The Hamiltonian becomes an MPO on L = $\log_2$N sites.
- For compressible geometry, χ is nearly size-independent.



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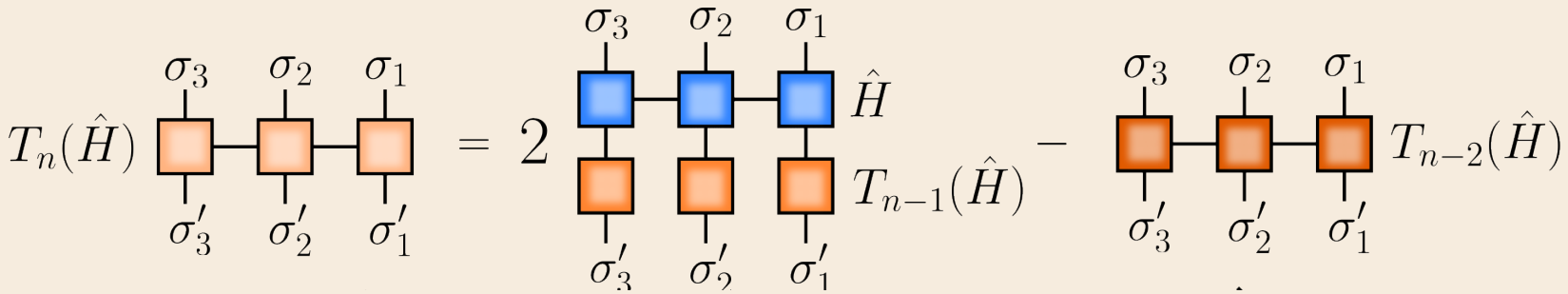
Extracting observables

Spectral function without diagonalization: KPM

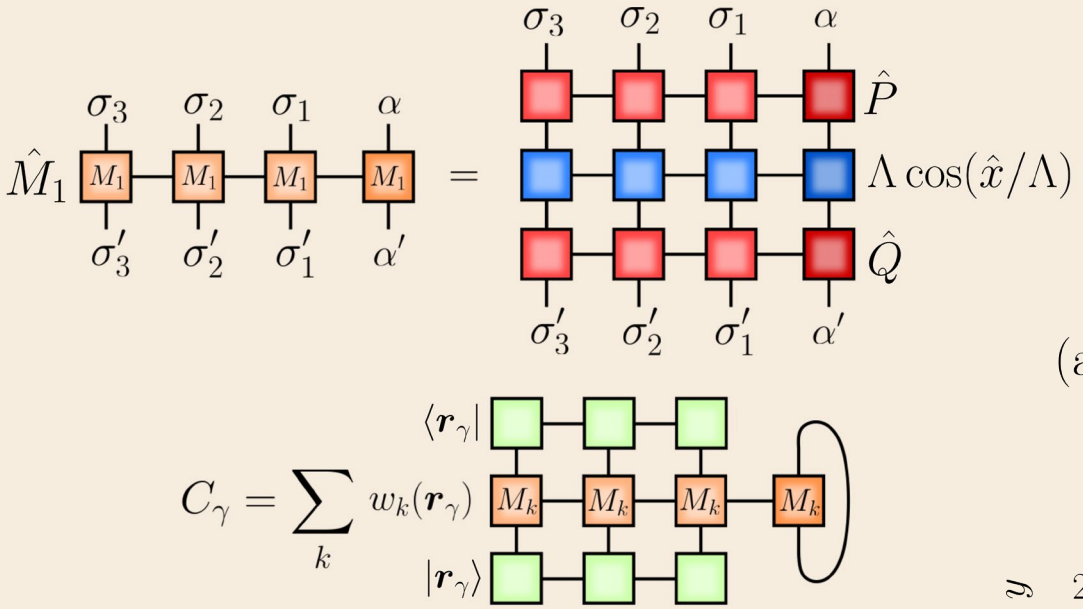
$$\hat{A}(\omega) \equiv \delta(\omega - \hat{H}) \approx \sum_{n=0}^{N_\mu} \frac{2 - \delta_{n0}}{\pi\sqrt{1-\omega^2}} g_n T_n(\hat{H}) T_n(\omega)$$

$$T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x)$$

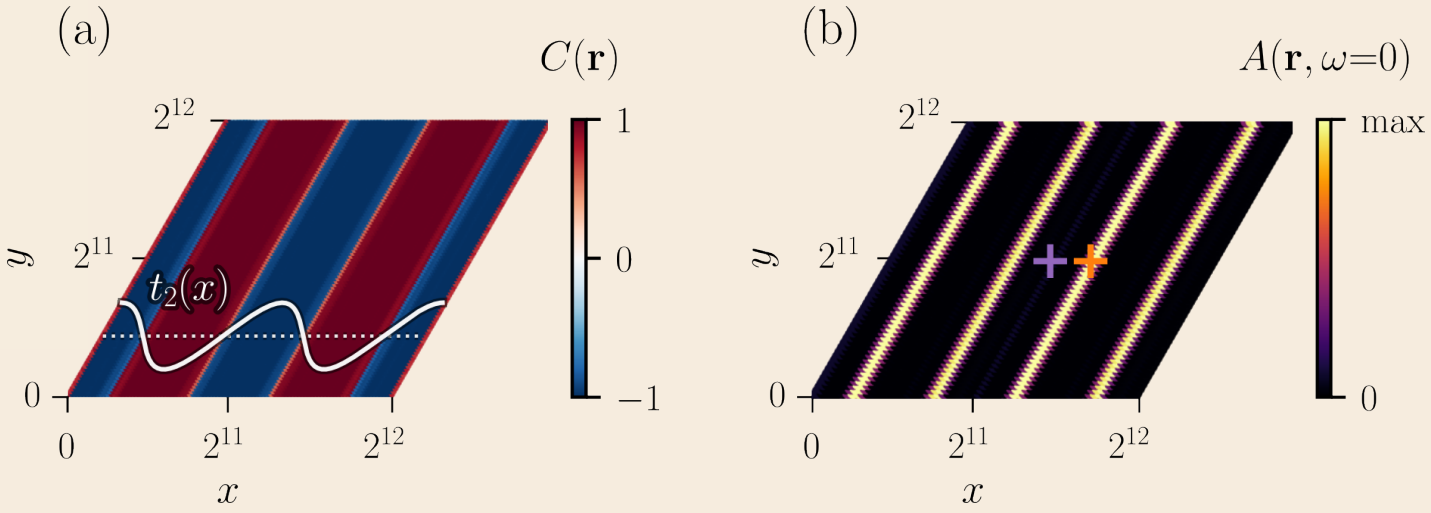


T. Antão, A. Moustaj, Y. Sun, J. Lado arXiv 2607.00991 (2026)

Band Topology



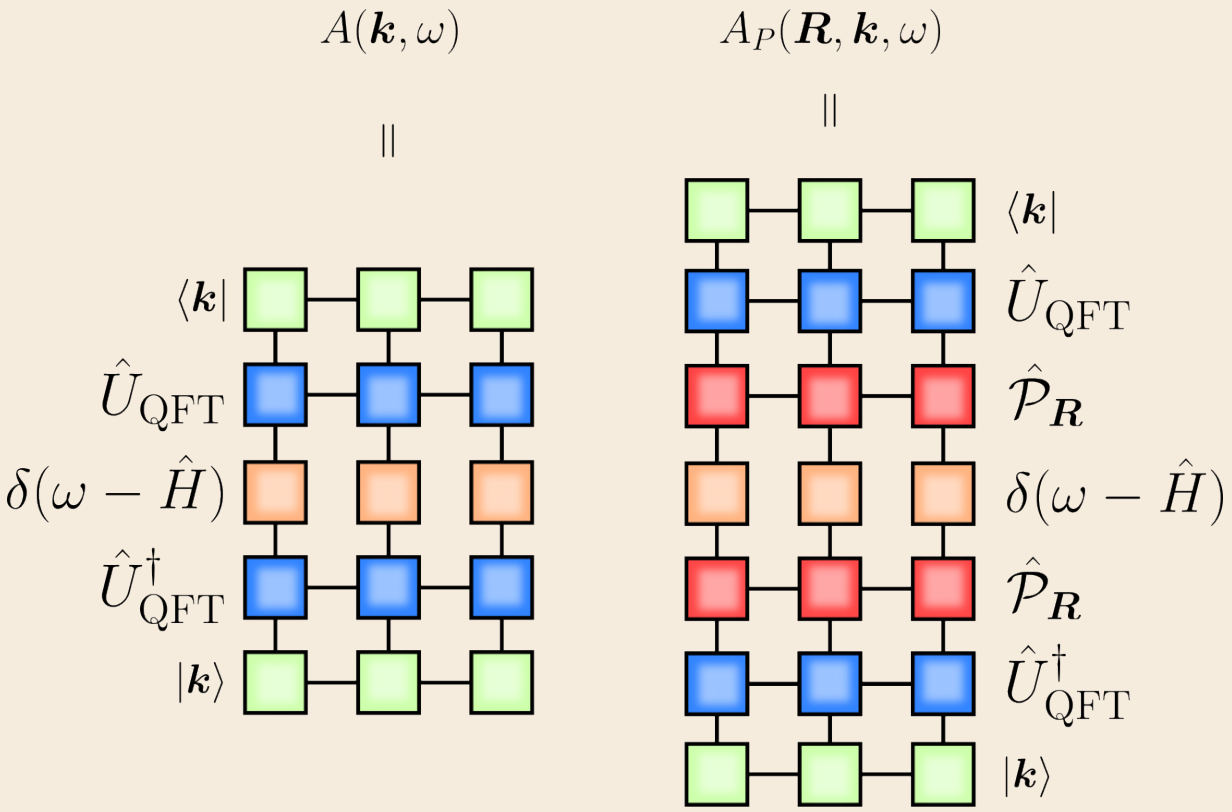
$$C(\mathbf{r}) = 4\pi i \langle \mathbf{r}| \hat{Q}\hat{x}\hat{P}\hat{y}\hat{Q} - \hat{P}\hat{x}\hat{Q}\hat{y}\hat{P} |\mathbf{r}\rangle$$

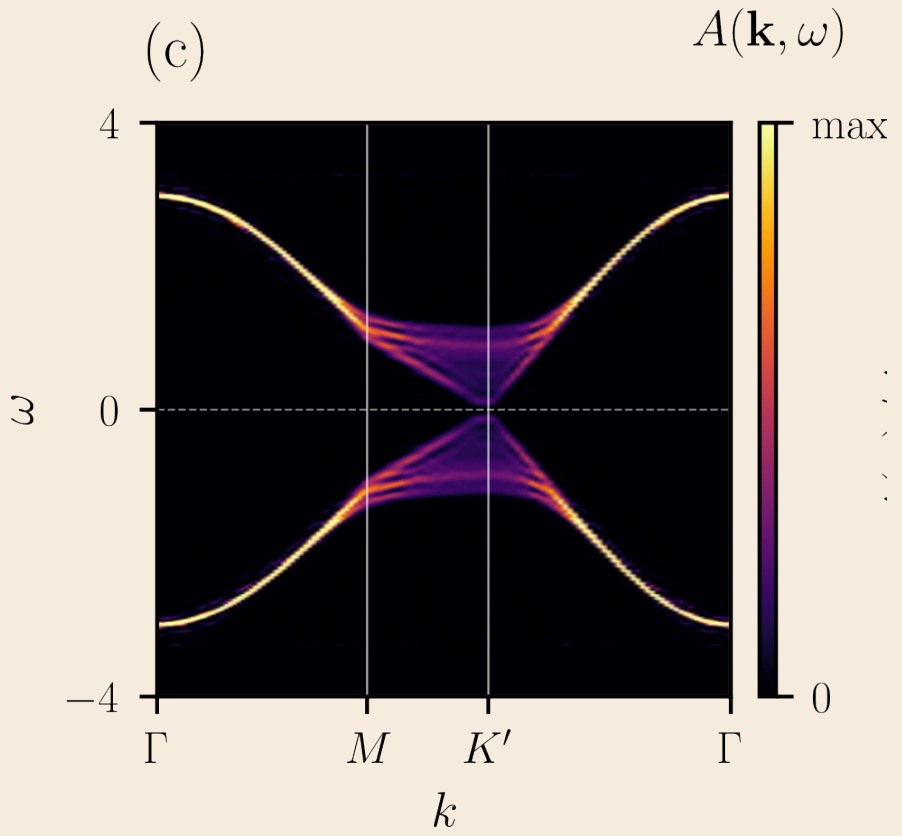


T. Antão, Y. Sun, A. Fumega, J. Lado PRL **136**, 156601 (2026)

T. Antão, A. Moustaj, Y. Sun, J. Lado arXiv 2607.00991 (2026)

Band Structures

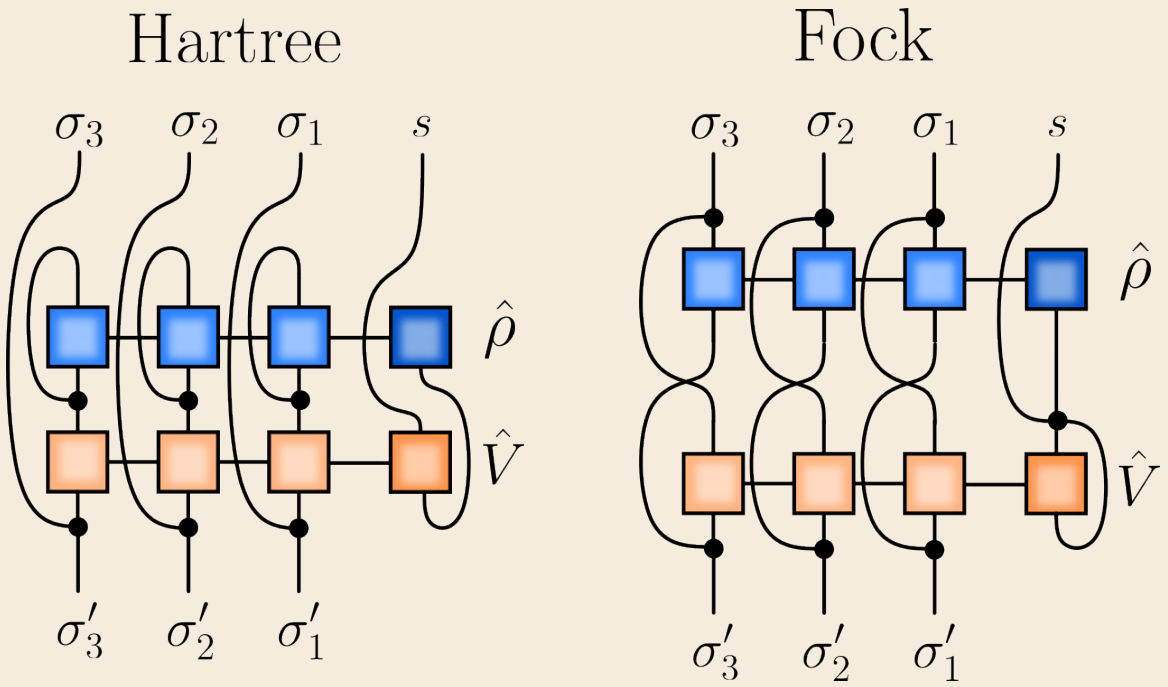


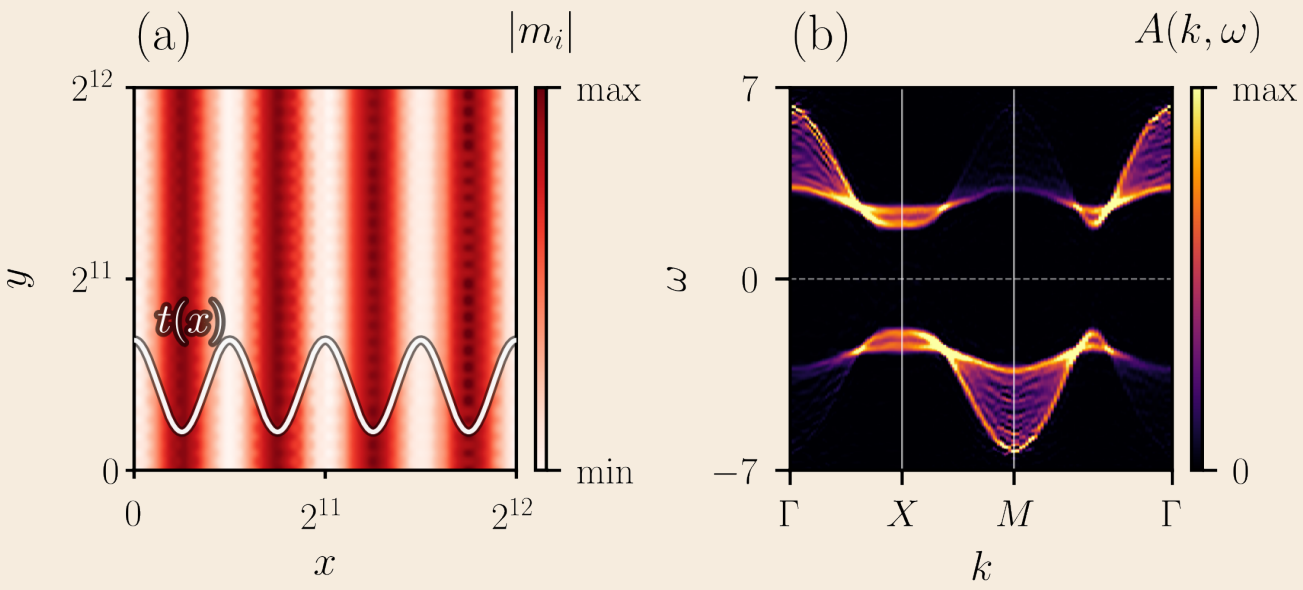


A. Moustaj, Y. Sun, T. Antão, J. Lado, PRR **8**, 023282 (2026)

T. Antão, A. Moustaj, Y. Sun, J. Lado, arXiv 2607.00991 (2026)

Self-Consistent Mean Field





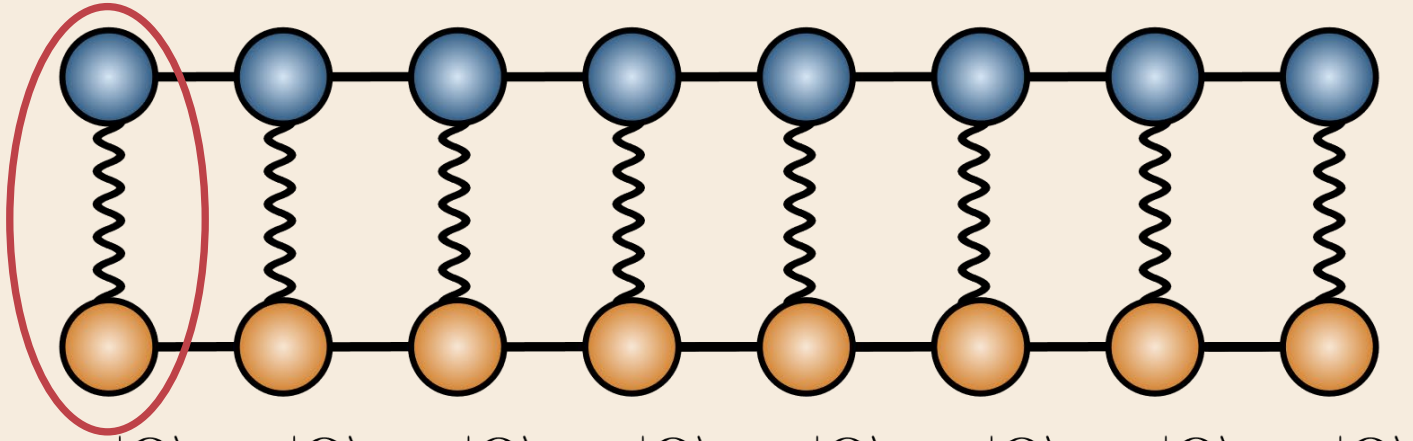
The Bethe-Salpeter-Equation Hamiltonian

A simple exciton system

Electrons:

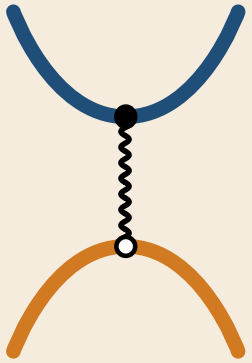
Holes:

$$c^\dagger_{c,1}|\Omega\rangle\ c^\dagger_{c,2}|\Omega\rangle\ c^\dagger_{c,3}|\Omega\rangle\ c^\dagger_{c,4}|\Omega\rangle\ c^\dagger_{c,5}|\Omega\rangle\ c^\dagger_{c,6}|\Omega\rangle\ c^\dagger_{c,7}|\Omega\rangle\ c^\dagger_{c,8}|\Omega\rangle$$



$$c_{v,1}|\Omega\rangle\ c_{v,2}|\Omega\rangle\ c_{v,3}|\Omega\rangle\ c_{v,4}|\Omega\rangle\ c_{v,5}|\Omega\rangle\ c_{v,6}|\Omega\rangle\ c_{v,7}|\Omega\rangle\ c_{v,8}|\Omega\rangle$$

- Only on-site interaction



A. Moustaj, Y. Sun, T. Antão, L.Eek, J. Lado, arXiv 2603.02011 (2026)

T. Antão, A. Moustaj, Y. Sun, J. Lado arXiv 2607.00991 (2026)

Hamiltonian in Operator Form

$$\hat{H} = \sum_{b\in\{c,v\}} \sum_{i,j} \left(t_{b,ij} + V_{b,i}\delta_{ij}\right) c^{\dagger}_{b,i} c_{b,j} + \sum_{i} U_i c^{\dagger}_{c,i} c_{c,i} c^{\dagger}_{v,i} c_{v,i}$$

b: band index
i, j: site index

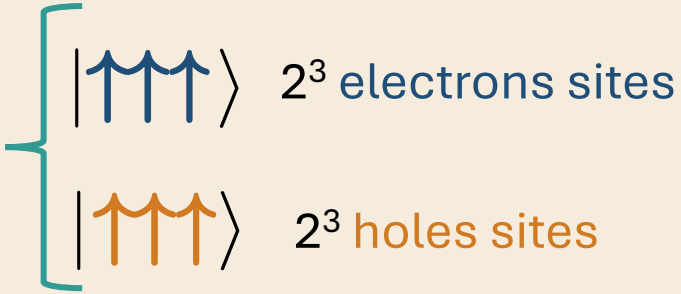
$$|l,m\rangle = c^{\dagger}_{c,l} c_{v,m} |\Omega\rangle \quad \Longrightarrow \quad [H_{\mathrm{X}}]_{l,m;l'm'} = \langle l,m| \hat{H} |l',m'\rangle$$

$$\hat{H}_{\mathrm{X}} = \hat{T}_c \otimes \hat{1} - \hat{1} \otimes \hat{T}_v - \hat{U}_{\mathrm{X}}$$

The pseudo-spin (quantics) representation

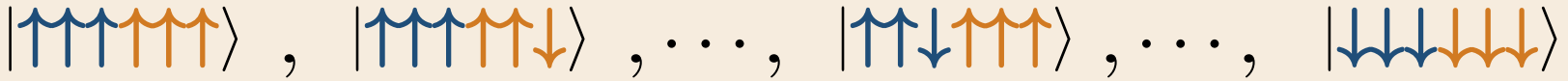
Assume one has a system of N = 8 = 2^3 physical sites:

Pseudo-spin representation:



$$c^\dagger_{c,1}c_{v,1}|\Omega\rangle\ ,\ c^\dagger_{c,1}c_{v,2}|\Omega\rangle\ ,\cdots,\ c^\dagger_{c,2}c_{v,1}|\Omega\rangle\ ,\cdots,\ c^\dagger_{c,8}c_{v,8}|\Omega\rangle$$

$$\updownarrow \text{Pseudo-spin encoding}$$

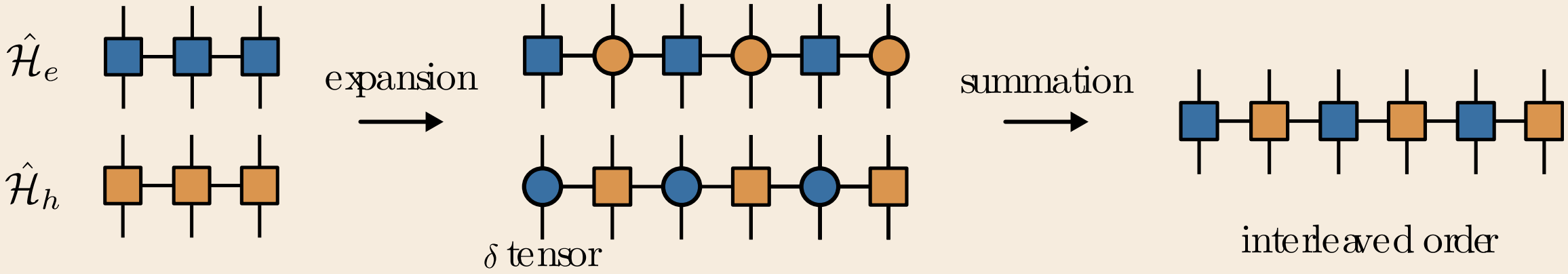


A. Moustaj, Y. Sun, T. Antão, L.Eek, J. Lado, arXiv 2603.02011 (2026)

Interleaving electrons and holes

INTERLEAVED ORDER

$$e_1 h_1 e_2 h_2 \cdots e_L h_L$$



A. Moustaj, Y. Sun, T. Antão, L.Eek, J. Lado, arXiv 2603.02011 (2026)

Spectral Observables: MPS propagation

Zero-size excitons in real space

$$\rho(\mathbf{r},\omega) = \langle \mathbf{r},\mathbf{r}|\, \delta(\omega - \hat{\mathcal{H}})\, |\mathbf{r},\mathbf{r}\rangle \approx \sum_{n=0}^{N_c} \frac{2-\delta_{n0}}{\pi\sqrt{1-\omega^2}} g_n \mu_n(\mathbf{r}) T_n(\omega)$$

Chebyshev moments

Kernel damping

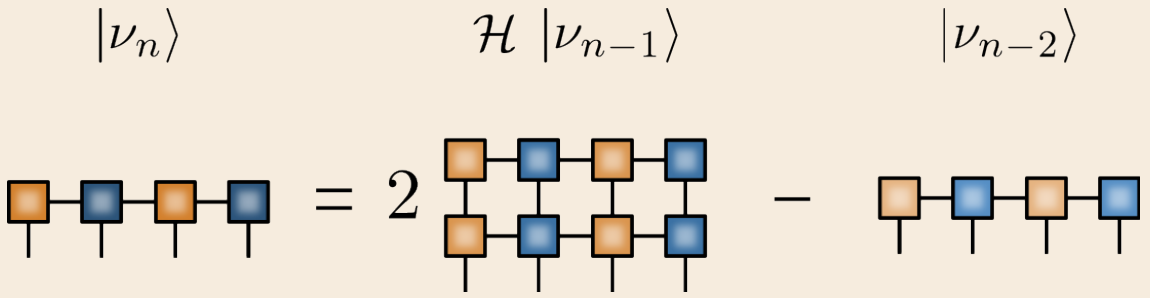
Chebyshev polynomials

$$\mu_n(\mathbf{r}) = \langle \mathbf{r},\mathbf{r}|\nu_n\rangle$$

$$|\nu_0\rangle = |\mathbf{r},\mathbf{r}\rangle$$

$$|\nu_1\rangle = \hat{H}\,|\nu_0\rangle$$

$\Rightarrow$

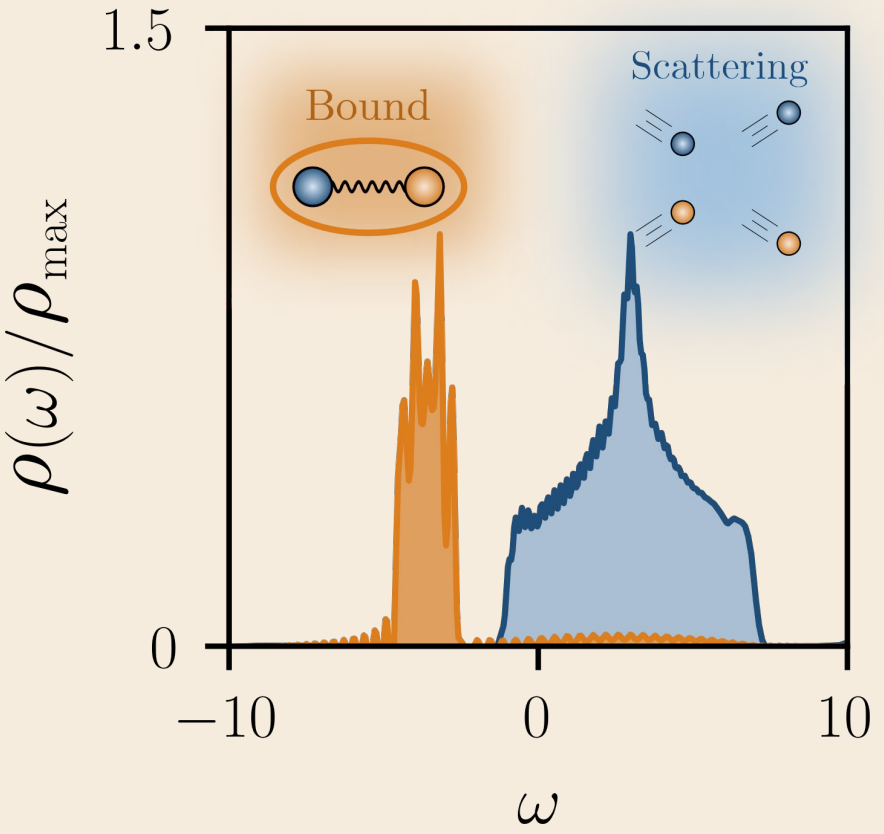


A. Moustaj, Y. Sun, T. Antão, L.Eek, J. Lado, arXiv 2603.02011 (2026)

Probing the exciton spectrum

Obtaining the full spectral signature without diagonalization

$$\rho(\omega) = \mathrm{Tr}\delta(\omega - \hat{\mathcal{H}})$$



T. Antão, A. Moustaj, Y. Sun, J. Lado arXiv 2607.00991 (2026)

Recap

$$\hat{H} = \underbrace{\hat{T}_c \otimes \hat{1}}_{\text{ELECTRON}} - \underbrace{\hat{1} \otimes \hat{T}_v}_{\text{HOLE}} - \underbrace{\hat{U}(\mathbf{r}_e, \mathbf{r}_h)}_{\text{INTERACTION}}$$

REAL-SPACE FUNCTIONS

V, t, U

→

QTCI COMPRESSION

MPS / diagonal MPO

→

INTERLEAVED SUM

2L-site BSE MPO

→

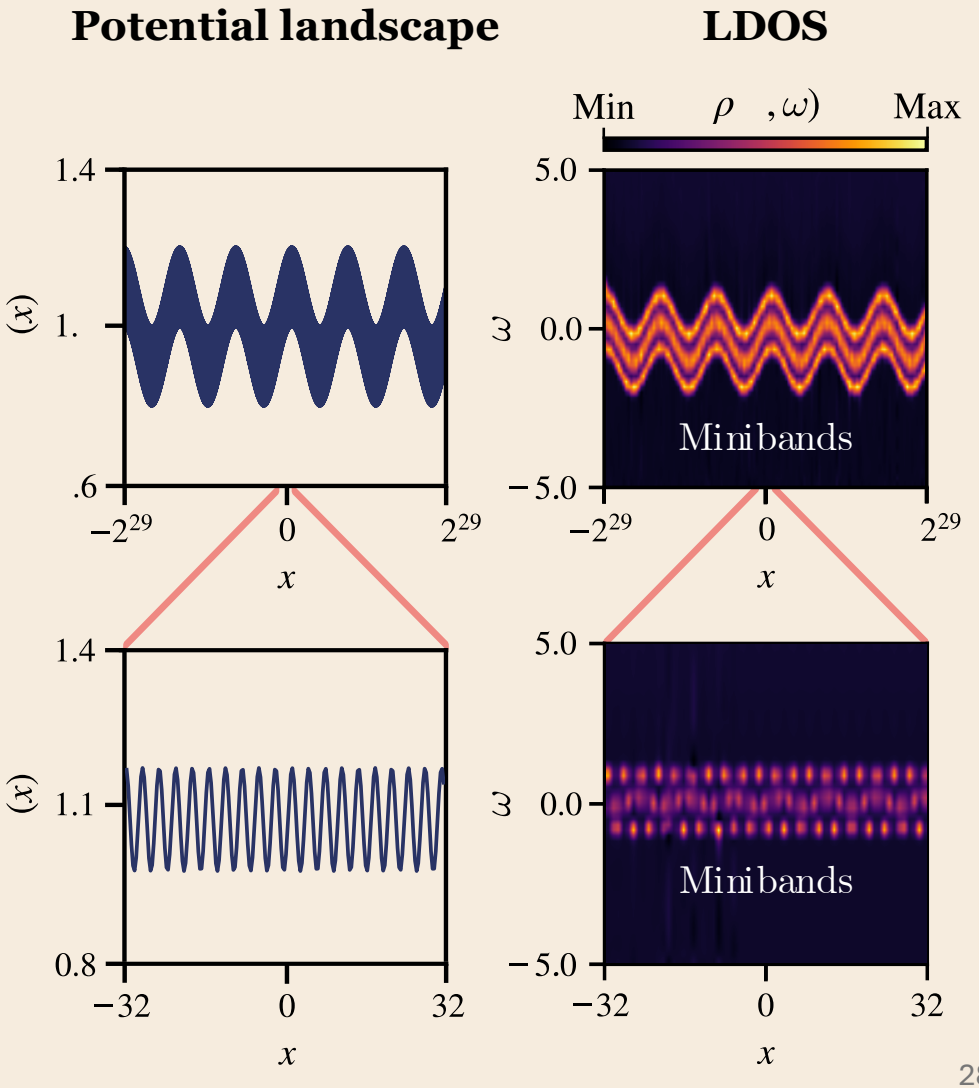
SPECTRA

MPS KPM

Results: 1D

> Atomic moiré potential and large-scale super-moiré potential

$$V_i = V_0 \left[1 + 0.1 \cos\left(\frac{\pi x_i}{3\sqrt{5}} \right) + 0.1 \cos\left(\frac{5\pi x_i}{N\sqrt{3}} \right) \right],$$



A. Moustaj, Y. Sun, T. Antão, L.Eek, J. Lado, arXiv 2603.02011 (2026)

Results: 2D

8-fold quasicrystalline potential at atomic and super-moiré scales

$$V(\mathbf{r}) = V_0 \left[1 + \sum_{n=1}^{4} \left(\Delta_\alpha \cos\left(\alpha \mathbf{k}_n \cdot \mathbf{r}\right) + \Delta_\beta \cos\left(\beta \mathbf{k}_n \cdot \mathbf{r}\right) \right) \right],$$

JACKSON

$N_\mu = 40$

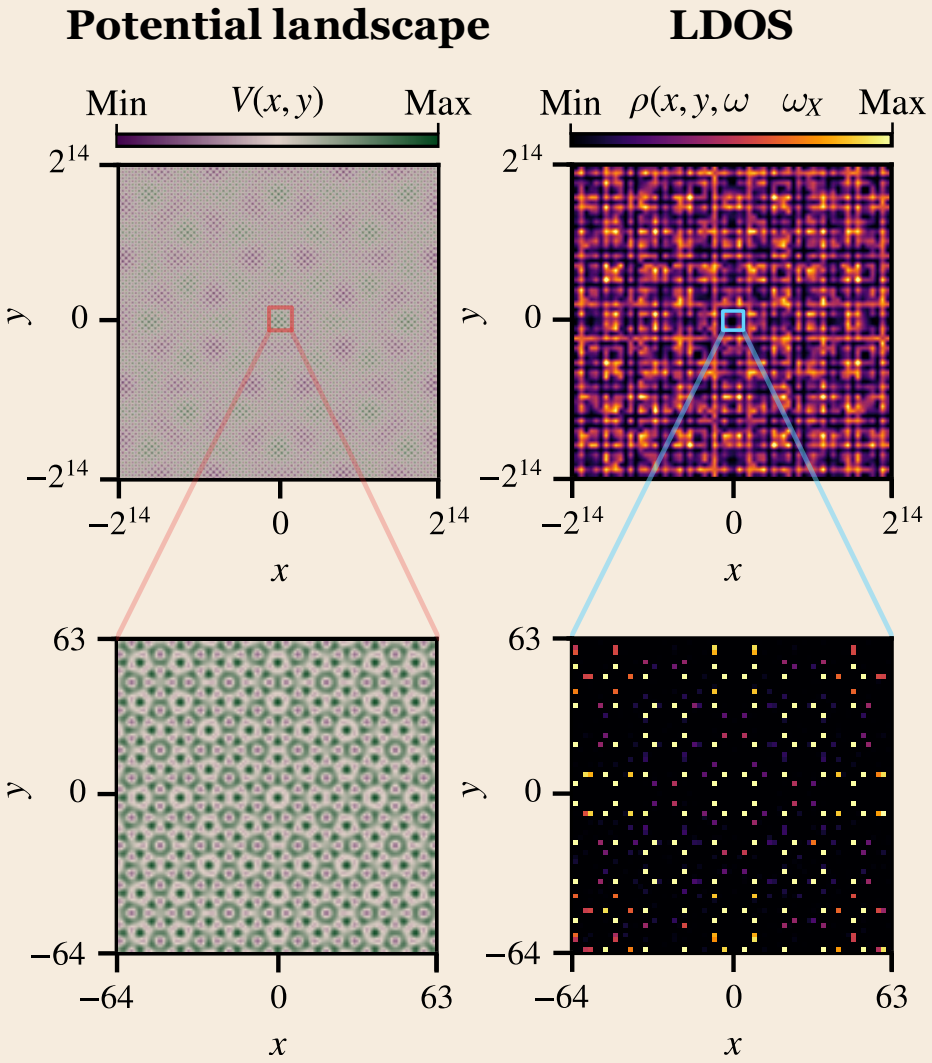
$\Delta E = 0.57$

HODC

$N_\mu = 40$

$\Delta E = 0.22$

≈ 2.6× sharper



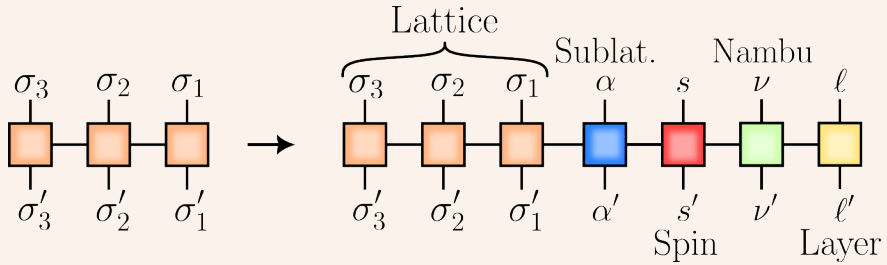
A. Moustaj, Y. Sun, T. Antão, L.Eek, J. Lado, arXiv 2603.02011 (2026)

Outlook

MORE REALISTIC INTERACTIONS

- Long-range Coulomb
- Exchange terms

INTERNAL STRUCTURE



BETTER 2D ARCHITECTURES

- Tree tensor networks for larger moment counts
- Beyond KPM strategies (leverage TN algorithms)

INTEGRATING OTHER METHODS

- Integration with DFT?
- Integration with RPA and GW?

T. Antão, A. Moustaj, Y. Sun, J. Lado arXiv 2607.00991 (2026)

Acknowledgement

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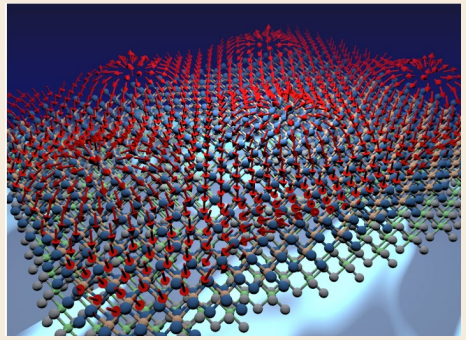
School of Science



CQM group

Yitao Sun

Tiago Antão

Lumen Eek

Jose Lado

TensorBinding.jl

https://github.com/TensorBinding/TensorBinding.jl

Take-Home

TensorBinding

COMPRESSION

Compressed Tight-Binding Methodology for single-particle and interacting two-particle systems using TN

LARGE-SCALE EXCITON SIMULATION

Exciton Simulations on system sizes beyond 10^9

SOME LIMITATIONS

Good scaling in 1D

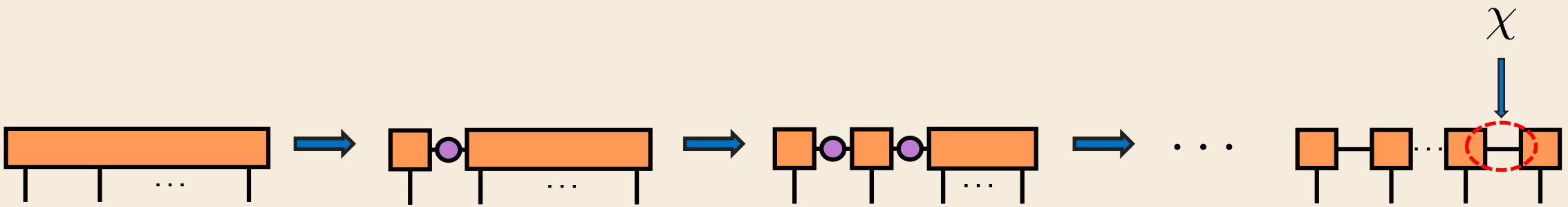
Currently limited resolution in 2D

REFERENCES

1. A. Moustaj, Y. Sun, T. Antão, L.Eek, J. Lado, arXiv 2603.02011 (2026)
2. T. Antão, A. Moustaj, Y. Sun, J. Lado arXiv 2607.00991 (2026)
3. T. Antão, Y. Sun, A. Fumega, J. Lado PRL **136**, 156601 (2026)
4. A. Moustaj, Y. Sun, T. Antão, J. Lado, PRR **8**, 023282 (2026)
5. Y. Sun, M. Niedermeier, T. Antão, A. Fumega, J. Lado, PRR **7**, 043288 (2025)
6. https://github.com/TensorBinding/TensorBinding.jl

Appendix

Tensor Trains – Efficient Approximators



Landscape of simulation tools

BerkleyGW

- First-principles (DFT input)
- Ab-initio screening
- High computational and memory cost

J. Deslippe et al., CPC **183**, 1269 (2012)

WanTIBEXOS

- Tight-Binding
- Material-oriented
- Cost NkNvNc

A. Dias et al., CPC **285**, 108636 (2023)

Xatu

- Tight-binding
- Theory-oriented
- Cost NkNvNc

A. Uría-Álvarez et al., CPC **295**, 109001 (2024)

PyMEX

- Tight-Binding
- Model screening
- Built for moiré
- Bloch Periodic
- Cost: NkNvNc
- Size reached: 1488 atoms reached

I. Maity et al., arXiv 2406.11098 (2025)

Quantics Representation of functions

Learning Feynman Diagrams with Tensor Trains

Yuriel Núñez-Fernández,[1,*] Matthieu Jeannin,[1] Philipp T. Dumitrescu,[2] Thomas Kloss,[1,3] Jason Kaye,[2,4] Olivier Parcollet,[2,5] and Xavier Waintal[1,†]

Tensorized orbitals for computational chemistry

Nicolas Jolly,[1] Yuriel Núñez Fernández,[2] and Xavier Waintal[1,*]
[1] *Université Grenoble Alpes, CEA, Grenoble INP, IRIG, PHELIQS, 38000 Grenoble, France*
[2] *Université Grenoble Alpes, CNRS, Institut Néel, 38000 Grenoble, France*

Solving the Gross-Pitaevskii equation on multiple different scales using the quantics tensor train representation

Marcel Niedermeier,[1,2] Adrien Moulinas,[2] Thibaud Louvet,[2] Jose L. Lado,[1] and Xavier Waintal[2]
[1] *Department of Applied Physics, Aalto University, 02150 Espoo, Finland*
[2] *Univ. Grenoble Alpes, CEA, Grenoble INP, IRIG, Pheliqs, 38000 Grenoble, France*

Permutation of Tensor-Train Cores for Computing Moments on Stochastic Differential Equations

Kayo Kinjo[1*], Rihito Sakurai[2], Tatsuya Kishimoto[1], and Jun Ohkubo[1]

A Quantum Inspired Approach to Exploit Turbulence Structures

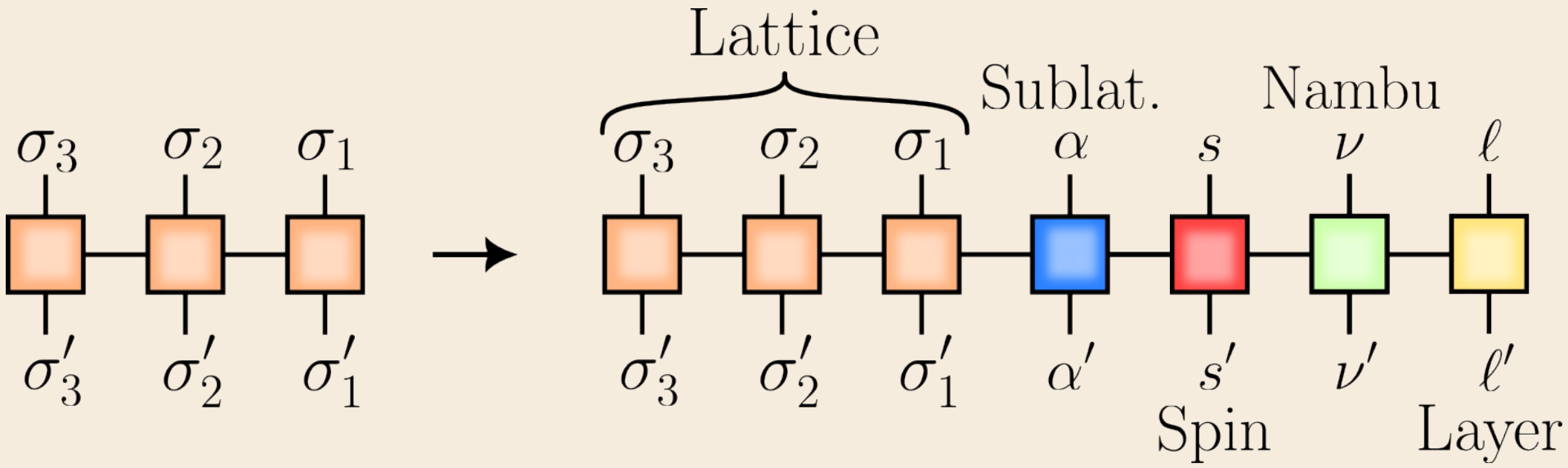
Nikita Gourianov[1],* Michael Lubasch[2], Sergey Dolgov[3], Quincy Y. van den Berg[1], Hessam Babaee[4], Peyman Givi[4], Martin Kiffner[5,1], and Dieter Jaksch[1,5,6†]

TENSOR TRAIN REPRESENTATIONS OF GREEKS FOR FOURIER-BASED OPTION PRICING OF MULTI-ASSET OPTIONS *

RIHITO SAKURAI†, KOICHI MIYAMOTO‡, AND TSUYOSHI OKUBO†§

... many more

Additional degrees of freedom: auxiliary indices



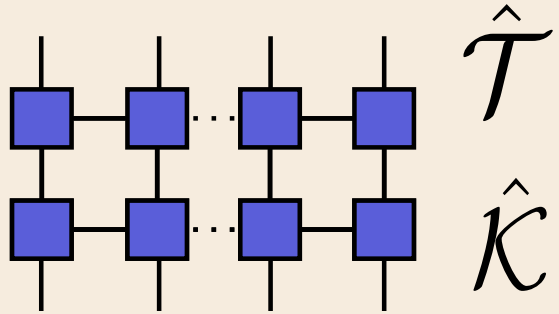
T. Antão, A. Moustaj, Y. Sun, J. Lado arXiv 2607.00991 (2026)

Tight-Binding Hamiltonians as Matrix Product Operators

$$\hat{K} = \sum_{ij} c_i^\dagger c_j \longrightarrow \hat{\mathcal{K}} = \sum_m \tau_m^+ \bigotimes_{n>m} \tau_n^- + \text{h.c}$$

$$t_{ij} \xrightarrow{\text{QTCI MPS}} |t\rangle \xrightarrow{\text{MPO}} \mathcal{T} = |t\rangle\langle t|$$

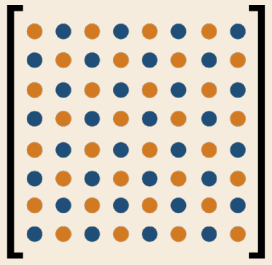
$$\hat{\mathcal{H}}_0 = \hat{\mathcal{T}}\hat{\mathcal{K}}$$



T. Antão, A. Moustaj, Y. Sun, J. Lado arXiv 2607.00991 (2026)

Compressing the Bethe-Salpeter Hamiltonian

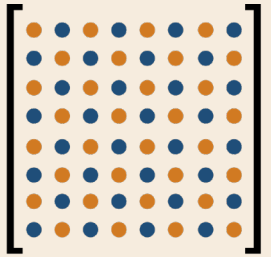
The goal: $\hat{H}_{\mathrm{X}} = \hat{T}_c \otimes \hat{1} - \hat{1} \otimes \hat{T}_v - \hat{U}_{\mathrm{X}}$



$2^{2L} \times 2^{2L}$
Matrix

$2L$ sites
Matrix Product Operator

or



$2^{2L} \times 2^{2L}$
Matrix

$2L$ sites
Matrix Product Operator

TN KPM LDOS: kernels

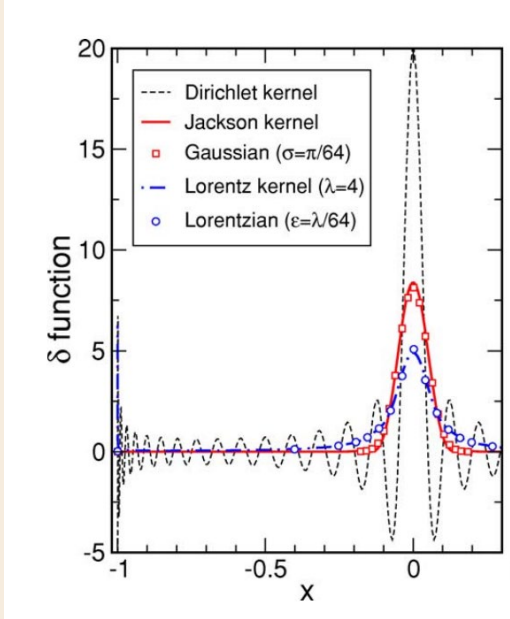
- Normally, we use the Jackson kernel

Introduces Gibbs Oscillations

$$\rho(\mathbf{x}, \tilde{E}) \approx \frac{1}{\pi\sqrt{1-\tilde{E}^2}}\left[g_0 + 2\sum_{n=1}^{N-1} g_n \mu_n(\mathbf{x}) T_n(\tilde{E})\right],$$

Damp them with the Jackson Kernel

$$g_n = \frac{(N-n+1)\cos\left(\frac{\pi n}{N+1}\right) + \sin\left(\frac{\pi n}{N+1}\right)\cot\left(\frac{\pi}{N+1}\right)}{N+1}$$



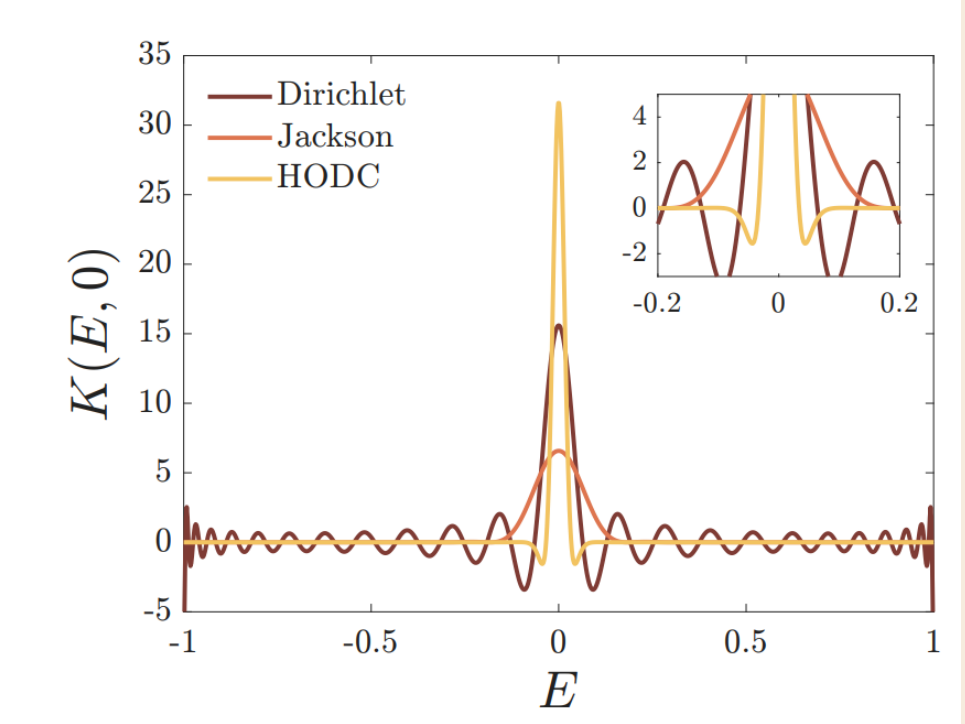
A. Weisse et al., RMP. **78**, 275 (2006)

TN KPM LDOS: HODC kernel

- Excitons: constrained to small # moments
- Need better convergence of KPM: HODC

$$K_\eta(\omega, E) = -\frac{1}{\pi}\sum_{l=1}^{m} \mathrm{Im}\,\frac{w_l}{\omega - E + \eta z_l}.$$

$$\mathcal{O}(\eta^m) \approx \mathcal{O}(1/N_\nu^m) \leq \mathcal{O}(1/N_\nu)$$



J. Yi et al., arXiv 2512.03149 (2025)

TN KPM LDOS: HODC kernel

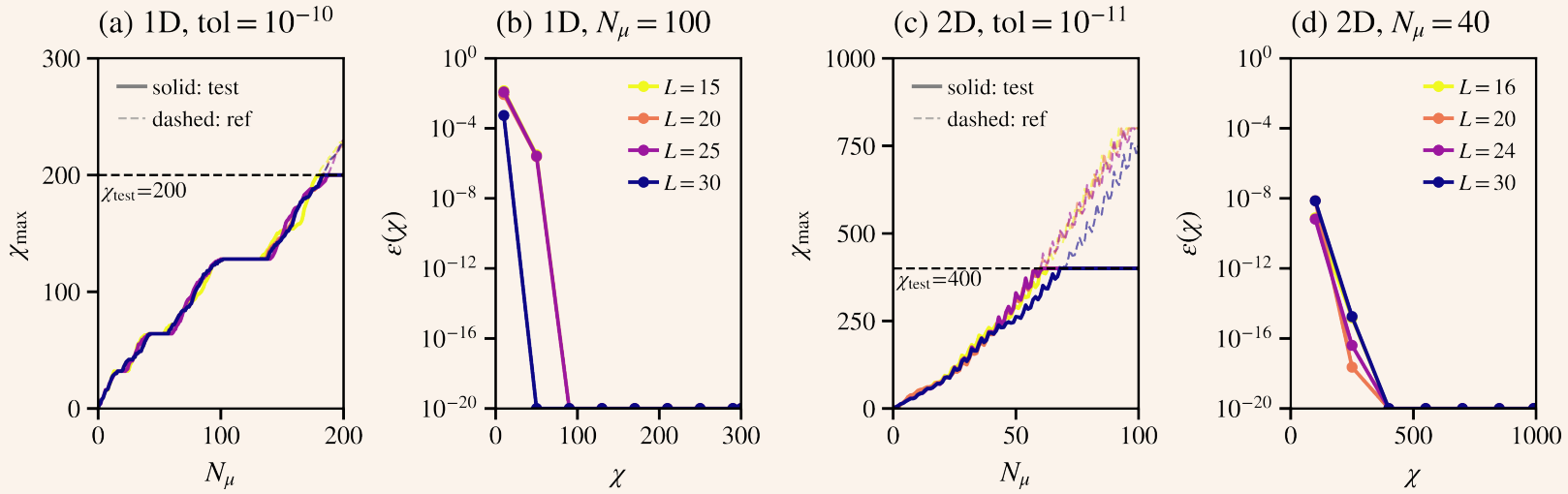
- Higher Order Delta Chebyshev kernel

$$\langle i|\,\delta(\omega - H)\,|i\rangle \approx \sum_{k=0}^{N_\nu - 1} \nu_k(\omega,\eta)\,\langle i|\,T_k\,(H)\,|i\rangle\,,$$

$$\nu_k(\omega,\eta) = \frac{2-\delta_{k0}}{n}\sum_{j=0}^{n-1} K_\eta(\omega, E_j)\cos\left(\frac{k(j+\frac{1}{2})\pi}{n}\right)$$

J. Yi et al., arXiv 2512.03149 (2025)

Limitations



1D

Accuracy floor by $\chi \lesssim 90$

2D

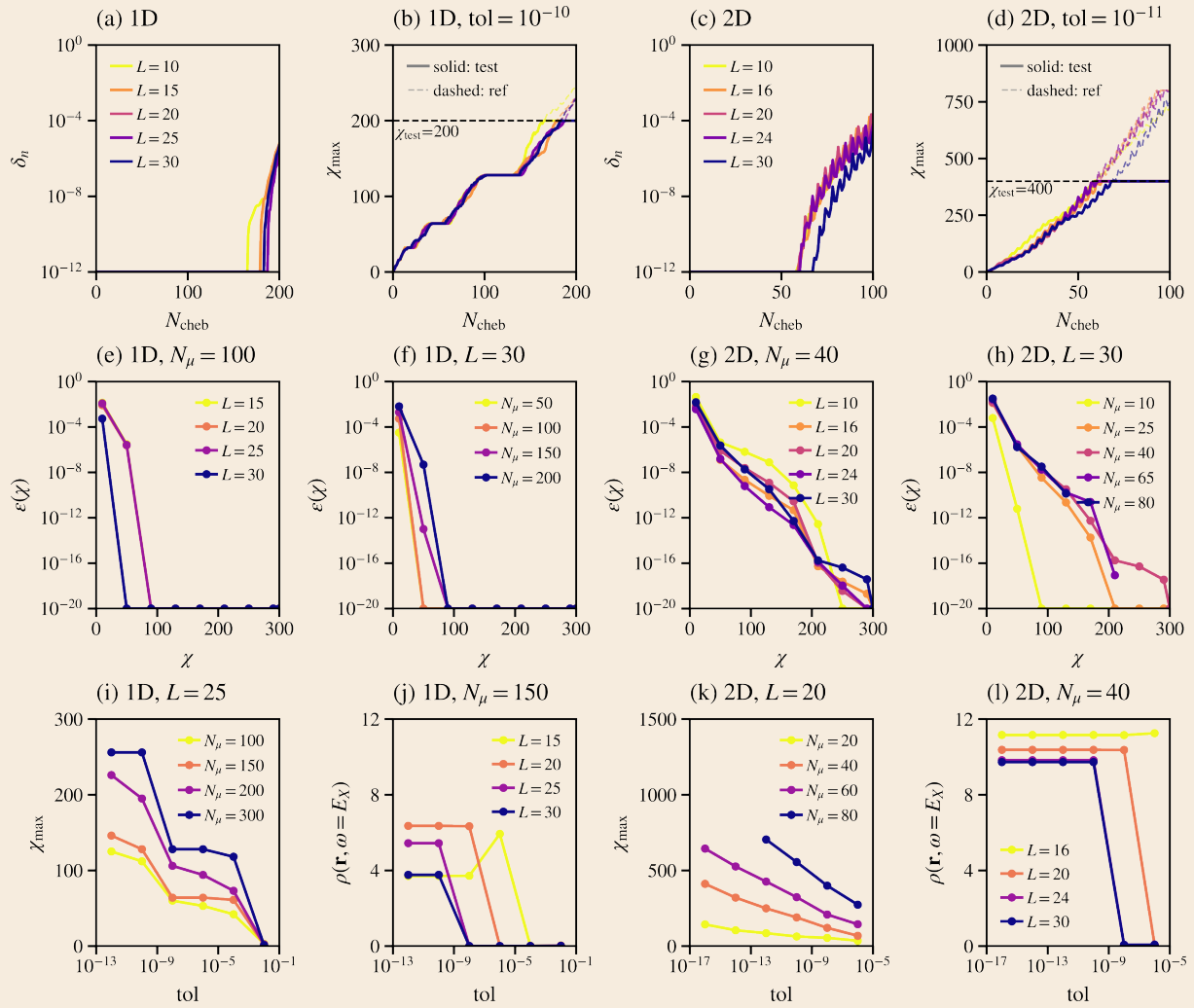
Accuracy floor near $\chi \approx 400$

MOMENT COUNT

2D hard beyond $N\mu \approx 60$

A. Moustaj, Y. Sun, T. Antão, L.Eek, J. Lado, arXiv 2603.02011 (2026)

Limitations



A. Moustaj, Y. Sun, T. Antão, L.Eek, J. Lado, arXiv 2603.02011 (2026)

Limitations

LIMIT	Outlook	Difficulty
Fast χ growth in 2D	Other network topologies	**Hard**
HODC non-positivity	Better architectures, more moments Alternative strategies to KPM	**Medium/Hard**
Minimal interaction model	Long-range and exchange kernels	**Implementation: easy** **Numerics: medium/hard?**