Multiscale space-time ansatz for correlation functions of quantum systems based on quantics tensor trains

arXiv:2210.12984v2 (to appear in PRX)

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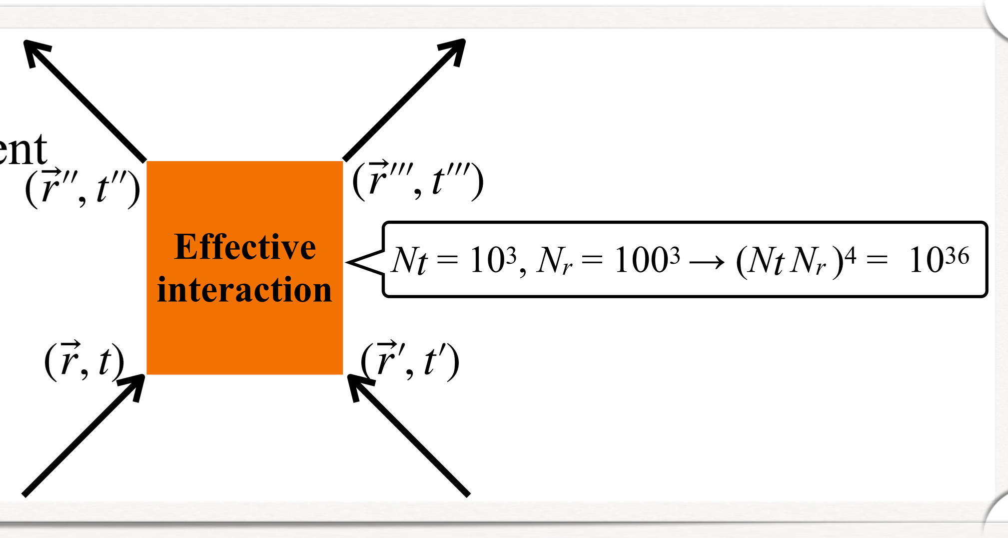
Background

Desired efficient numerical treatment of space-time dependence of correlation functions!

Quantum embedding, first-principles calculations

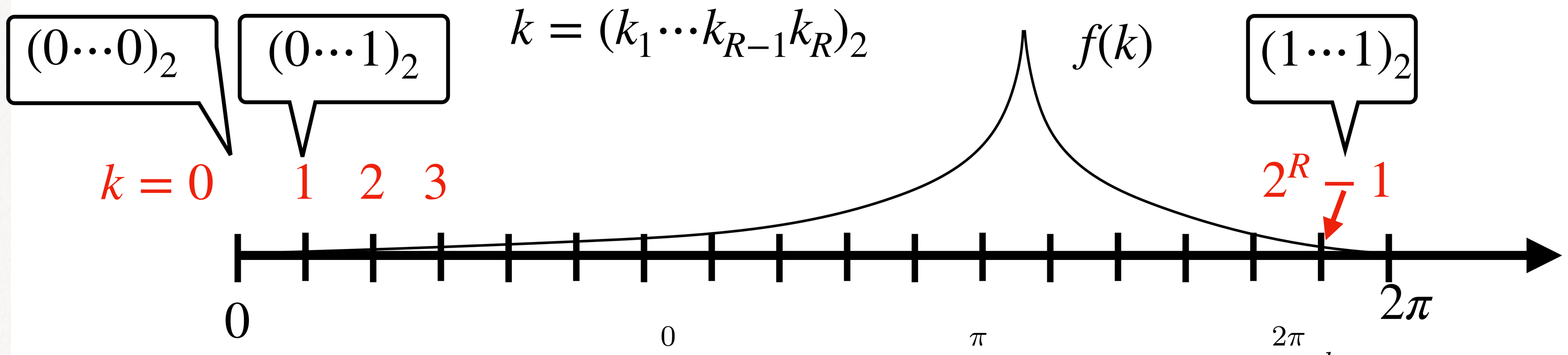


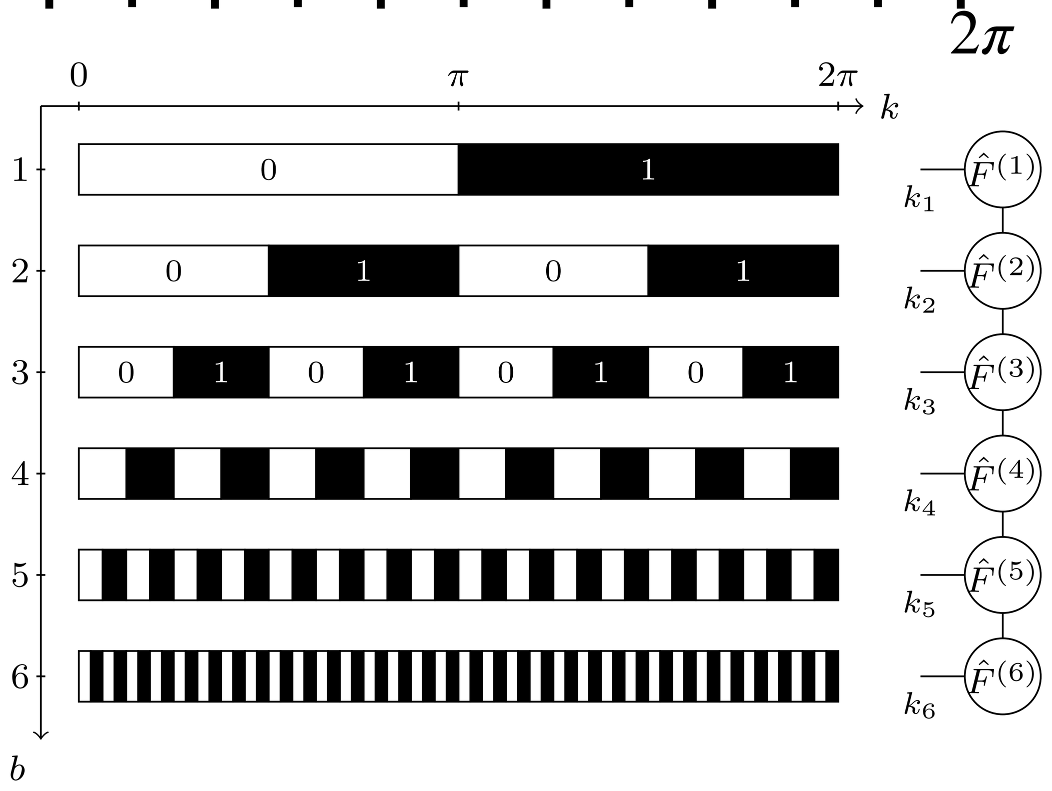
What's new

- Wide range of length scales in space-time
- Systematic control over truncation error
- Computation in compressed form
- Straightforward implementations as computer code

Quantics tensor trains (QTT)

I. V. Oseledets, Doklady Math. **80**, 653 (2009)
B. N. Khoromskij, Constr. Approx. **34**, 257 (2011)



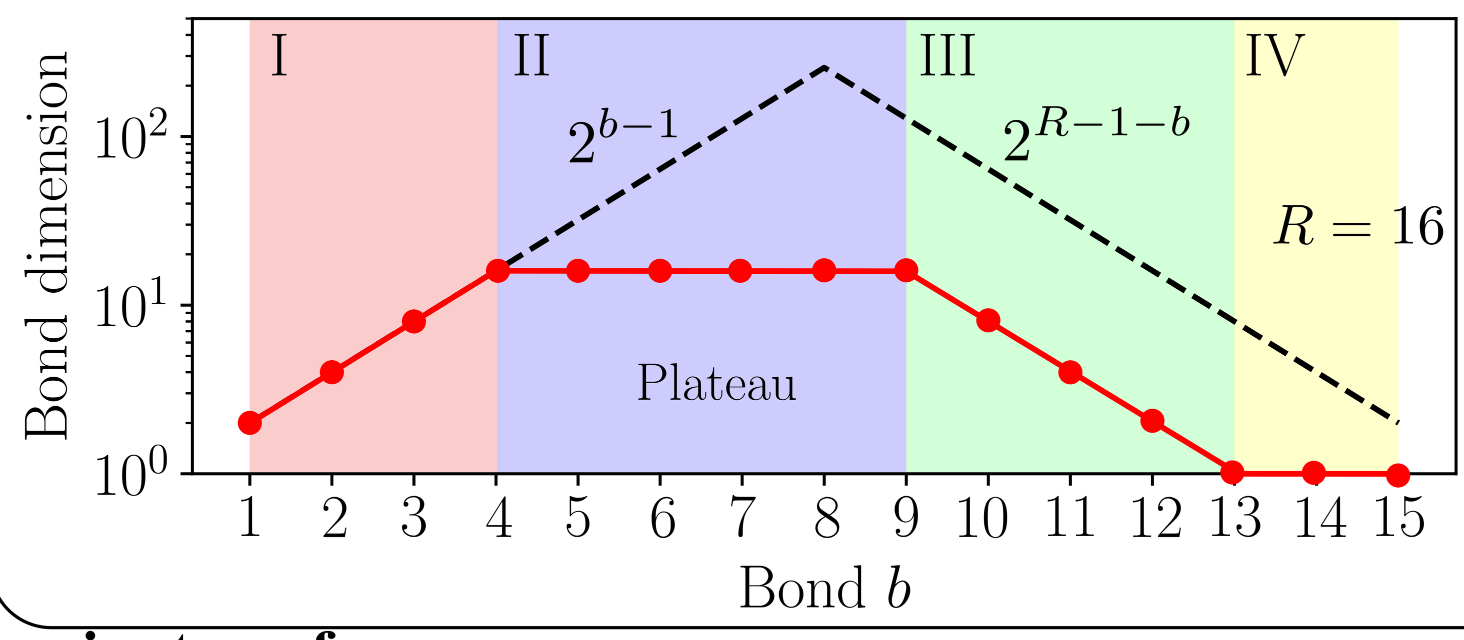


If QTT compressible, bond dimension $\ll 2^{R/2}$

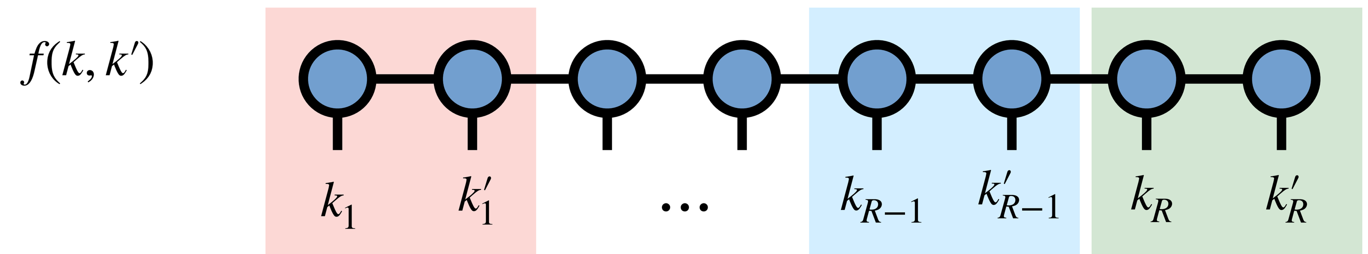
$$f(k_1, k_2, \cdots, k_R) \approx \sum_{\alpha_1=1}^{D_1} \cdots \sum_{\alpha_{R-1}=1}^{D_{R-1}} \hat{F}^{(1)}_{k_1,1\alpha_1} \hat{F}^{(2)}_{k_2,\alpha_1\alpha_2} \cdots \hat{F}^{(R)}_{k_R,\alpha_{R-1}1}$$

Tensor train/Matrix product state

Length-scale separation→Exponential advantage for storage!



Multivariate function

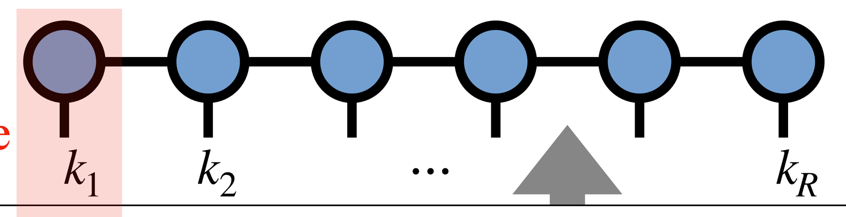


Same length scale

Fourier transform

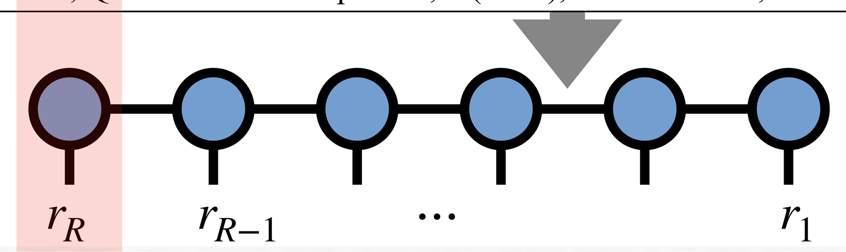
Coarse

Same length scale



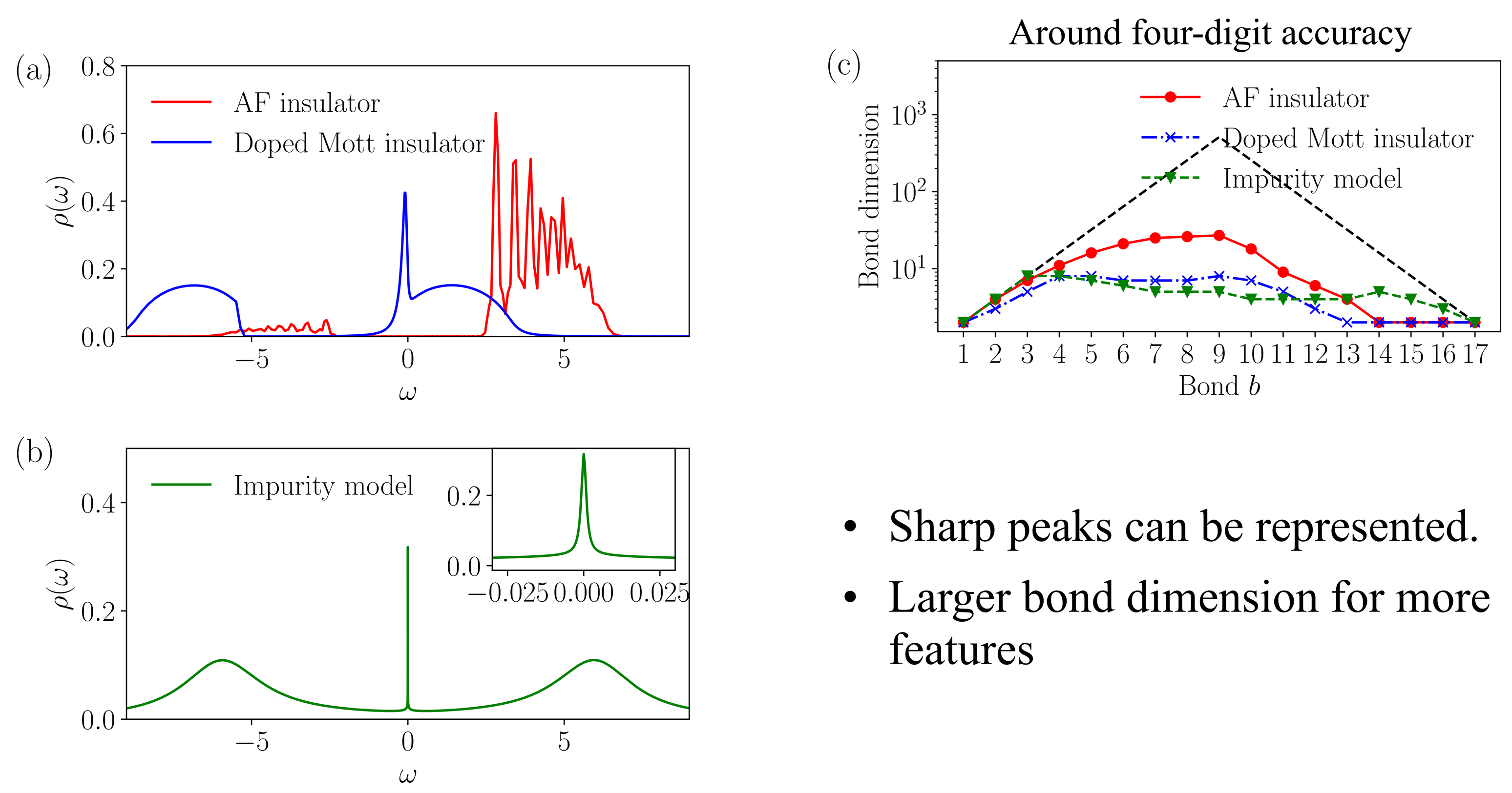
Matrix product operator (MPO) for Fourier transform has a small ($D < 20$).
K. J. Woolfe *et al.*, Quantum Inf. Comput. **17**, 1 (2017), J. Chen *et al.*, arXiv:2210.08468v1

Short range



$r = 0, 1, \cdots, 2^R - 1 = (r_1 \cdots r_{R-1} r_R)_2$

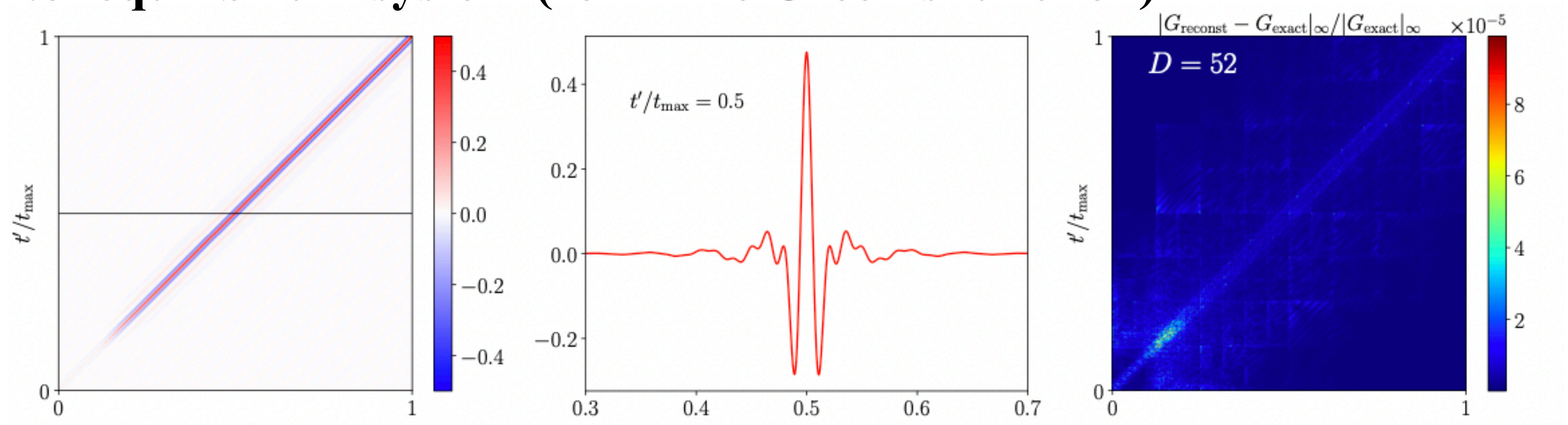
Compression



- Sharp peaks can be represented.
- Larger bond dimension for more features

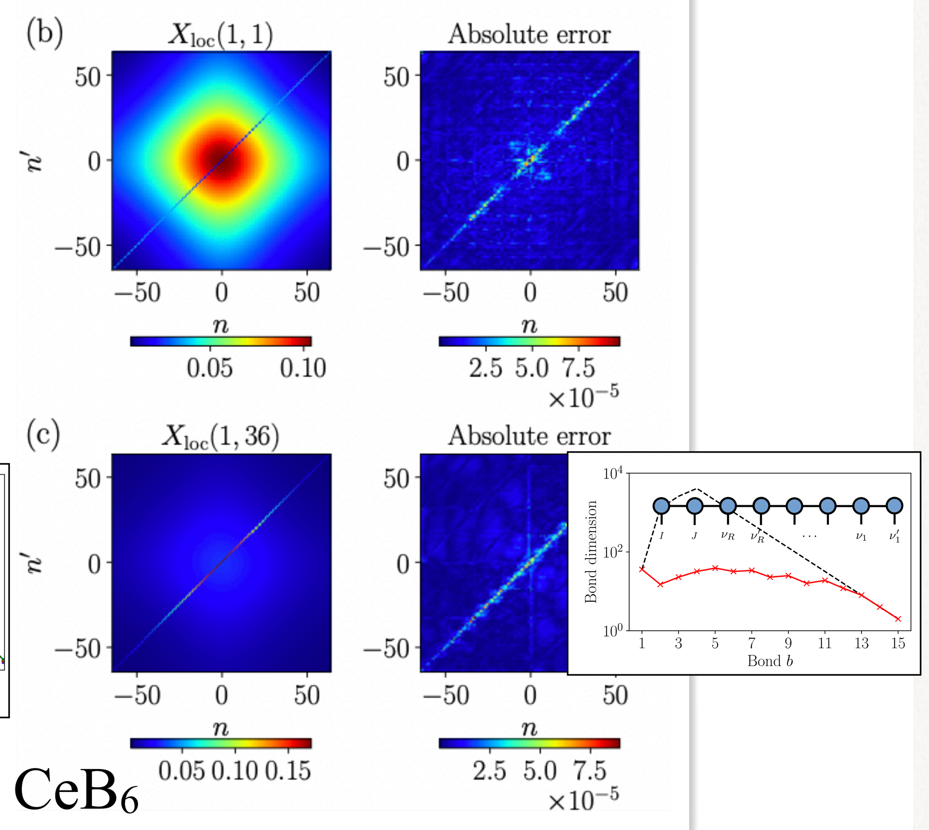
Nonequilibrium system (real-time Green's function)

Compression ratio ~ 10^3

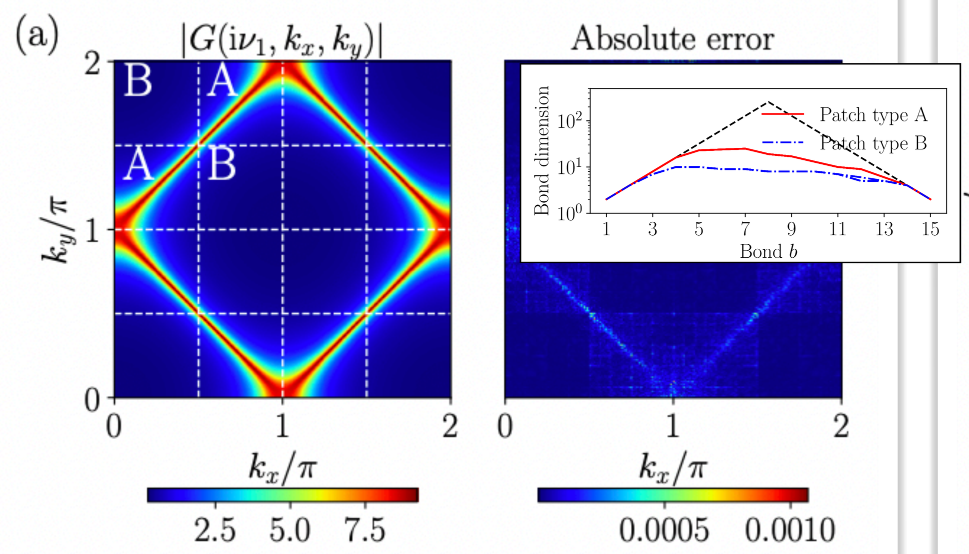


All QTT compressible!

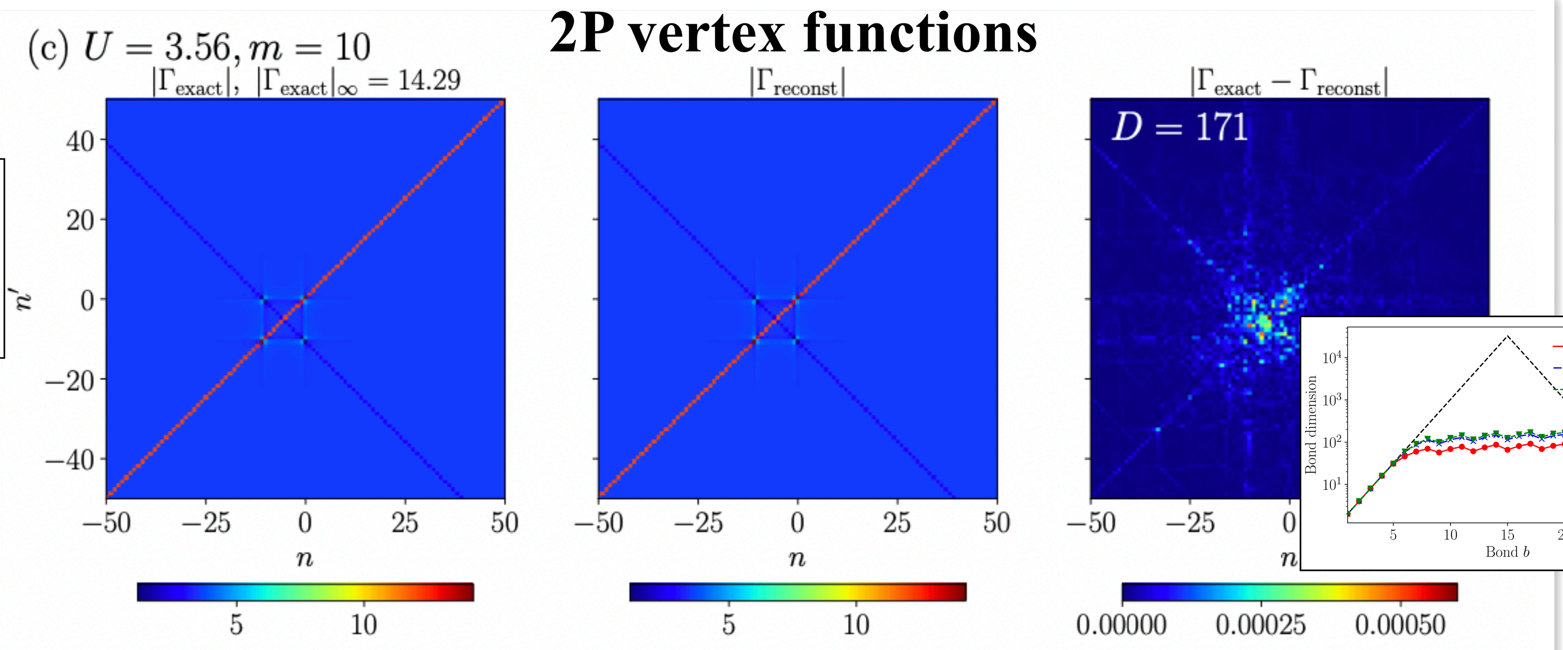
Multipolar susceptibility



1P momentum space



2P vertex functions



Computation

Exponential speed up!

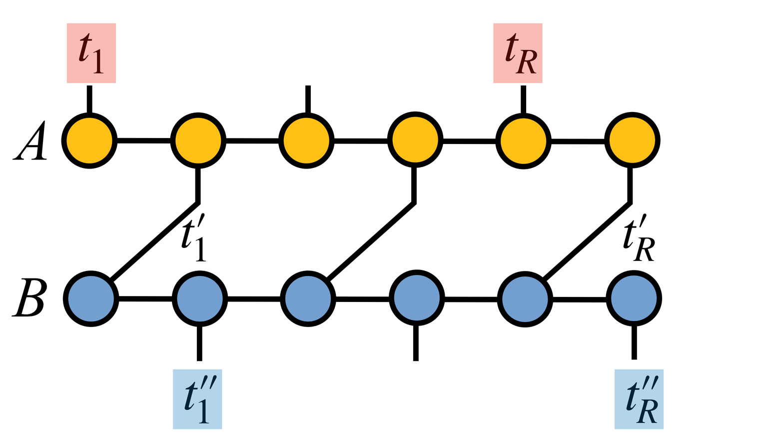
☑Fourier transform
☑Matrix multiplication
☑Dyson/Bethe-Salpeter equation

$$F = \Gamma + \Gamma X_0 F$$

➡ HS *et al.*, arXiv:2210.12984v2

$$C(t, t'') = \int \mathrm{d}t' A(t, t') B(t', t'')$$

$$C(t_1, t_1'', \cdots, t_R, t_R'') = \sum_{t_1', \cdots, t_R'} A(t_1, t_1', \cdots, t_R, t_R') B(t_1', t_1'', \cdots, t_R', t_R'')$$



➡ Quantics tensor cross interpolation
M. K. Ritter, Y. N. Fernández, M. Wallerberger, J. von Delft, HS, X. Waintal, arXiv:2303.11819