Tensorizing Feynman diagrams

Quantics tensor trains and quantics tensor cross interpolation

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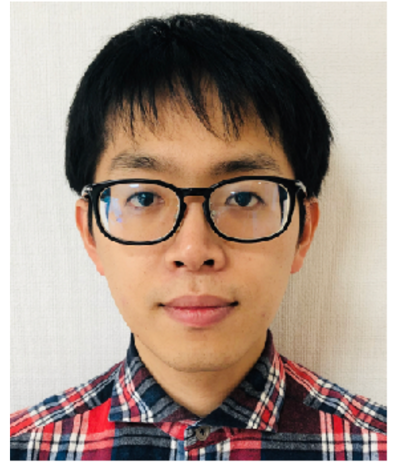
FY2023-2025 MEXT -KAKENHI- Grant-in-Aid for Transformative Research Areas (B)
“Computational materials science based on quantum-classical hybrid algorithms”

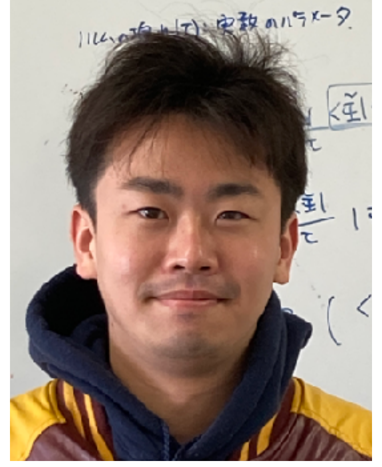
PRX **13**, 021015 (2023), arXiv:2303.11819

Collaborators

- HS *et al.*, PRX **13**, 021015 (2023)








M. Wallerberger **A. Kauch** **Y. Murakami** **K. Nogaki** **R. Sakurai** **P. Werner**

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- M. K. Ritter, Y. N. Fernández, M. Wallerberger, J. von Delft, HS, X. Waintal, arXiv:2303.11819




M. K. Ritter **J. von Delft** **Y. N. Fernández** **X. Waintal**

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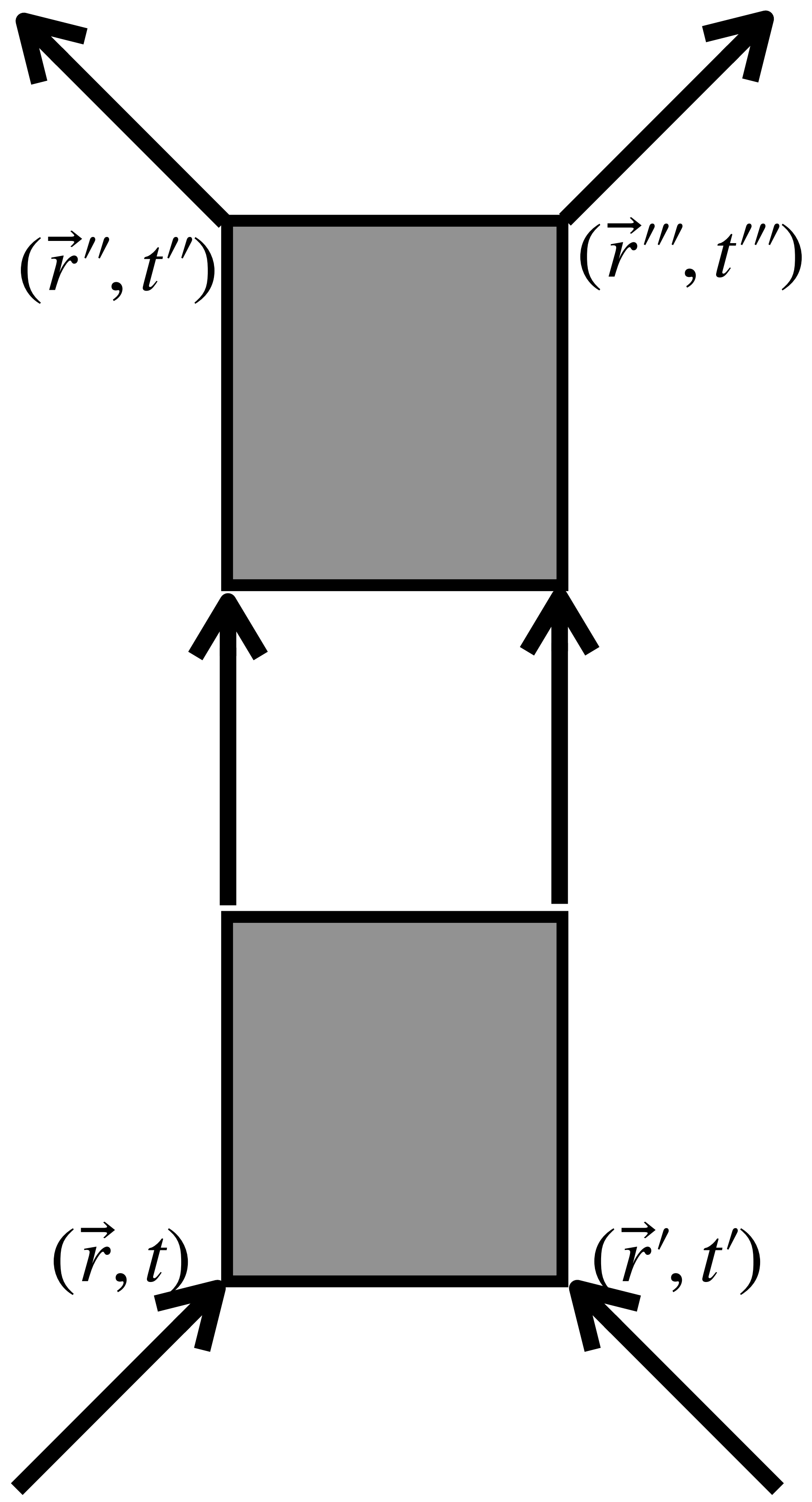
Special thanks to E. Miles Stoudenmire (CCQ) for his help in implementing our code with ITensors.jl

Tensors for all field theories!



"Quantics" allows

- Compression: Coexisting (exponentially) different length scales
- Computation: Integration, Fourier transform, convolution

Benchmarks: Solving Dyson/Bethe equations, BZ integration…

Beyond condensed matter physics!

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Outline

- Introduction
- Part I Quantics tensor train

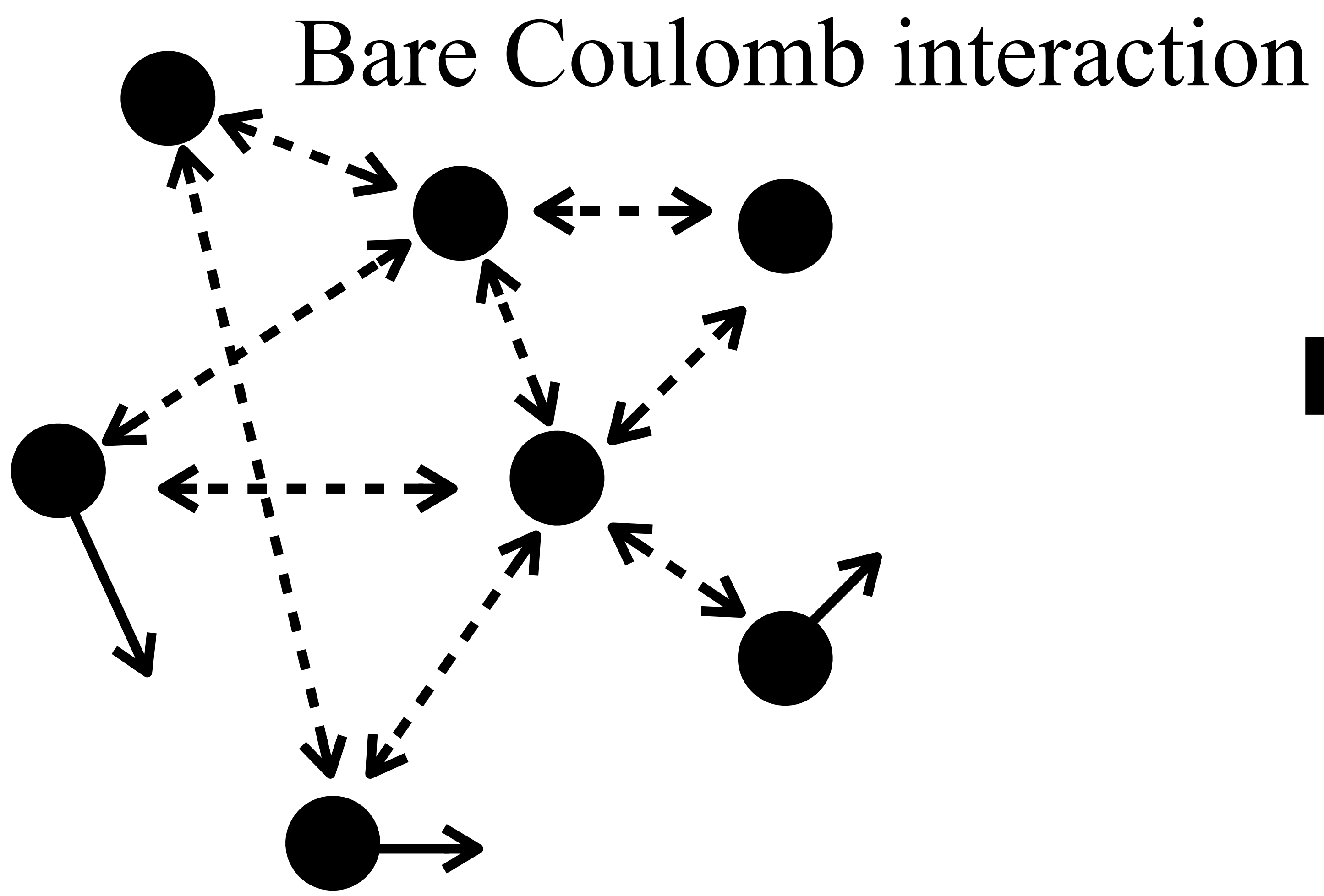
  HS *et al*., PRX **13**, 021015 (2023)
- Part II Quantics tensor cross interpolation

  M. K. Ritter, Y. N. Fernández, M. Wallerberger, J. von Delft, **HS**, X. Waintal, arXiv:2303.11819
- Outlook & summary

Quantum field theories

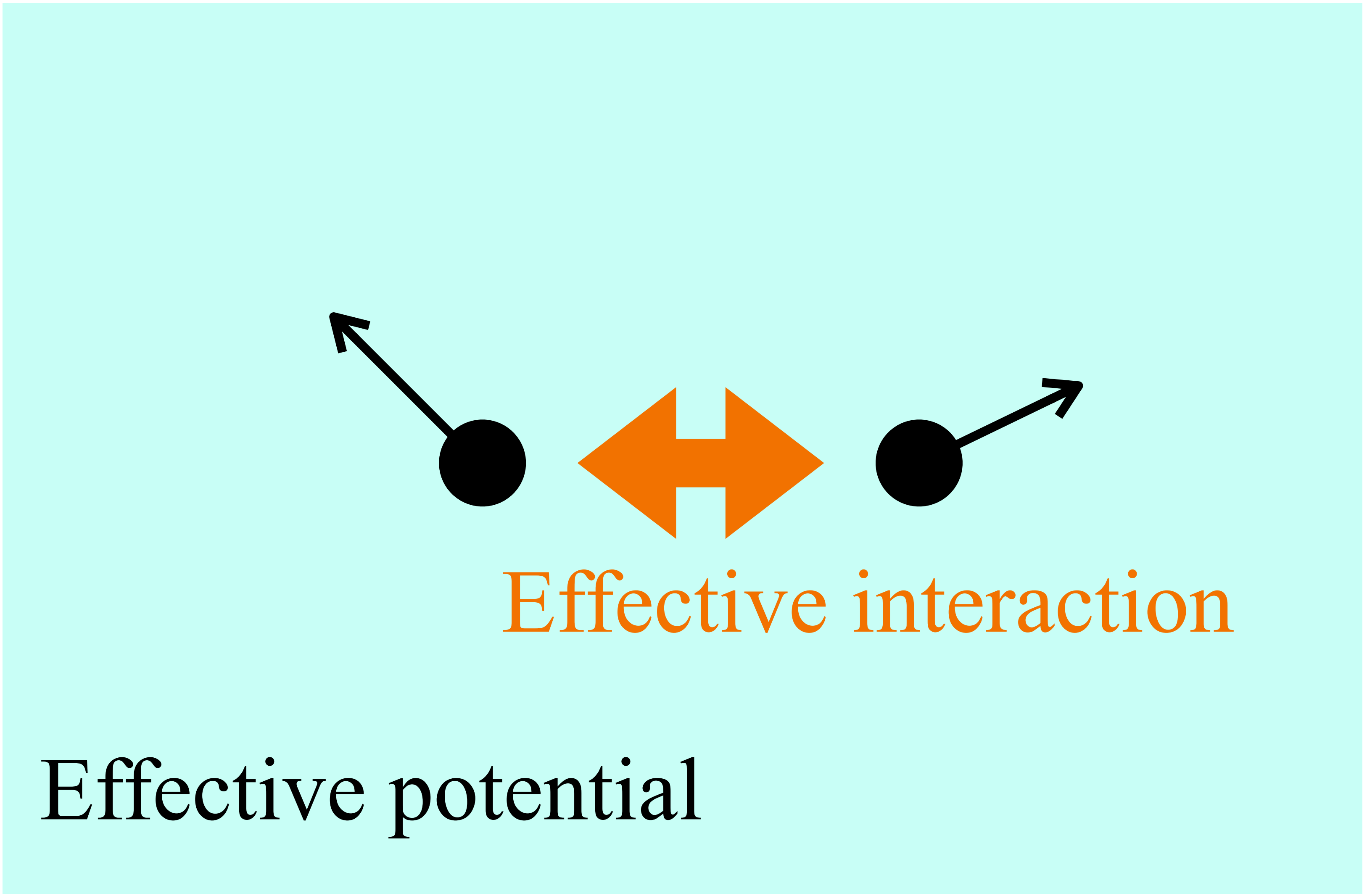
with a focus on many-body electronic systems

Many-particle interacting system



Exponential growth in computational cost

Effective few-particle system



DFT (Kohm-Sham), diagrammatic many-body theories, DMFT, *etc*.

Grand challenges

- More accurate mapping
- Still very expensive to solve effective few-particle systems

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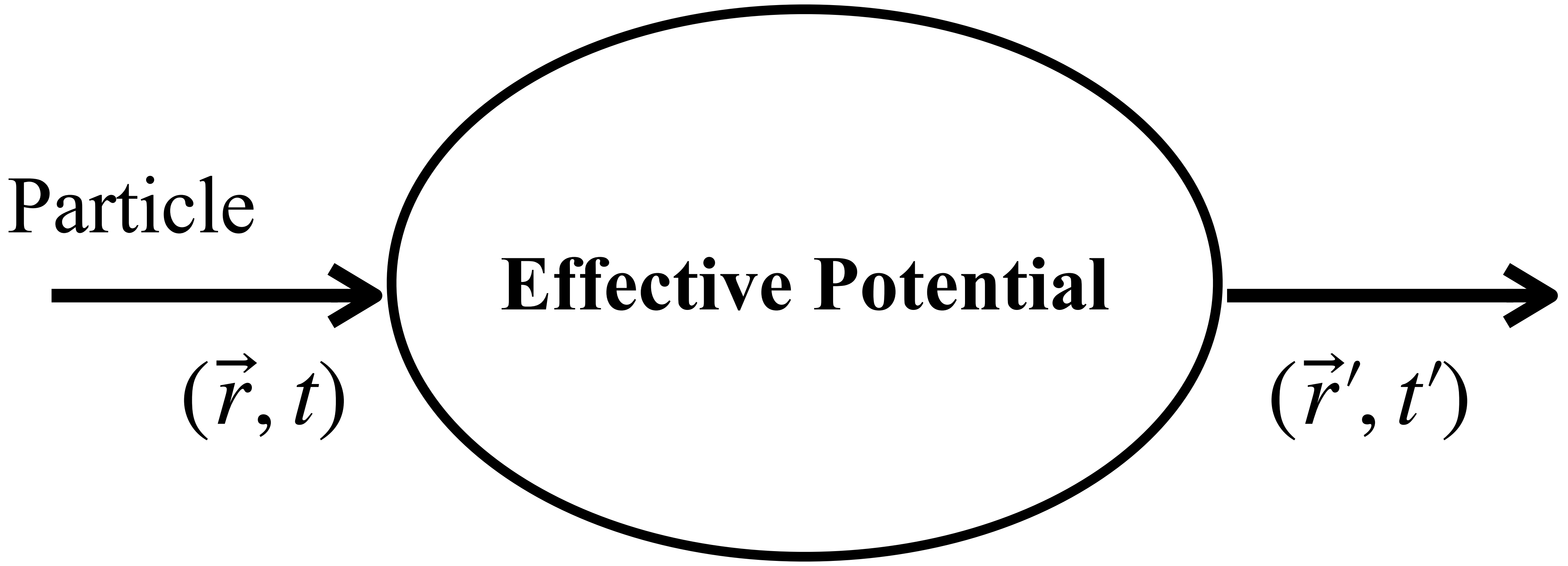
Building block of quantum field theory

Correlation functions in a high-dimensional space-time domain

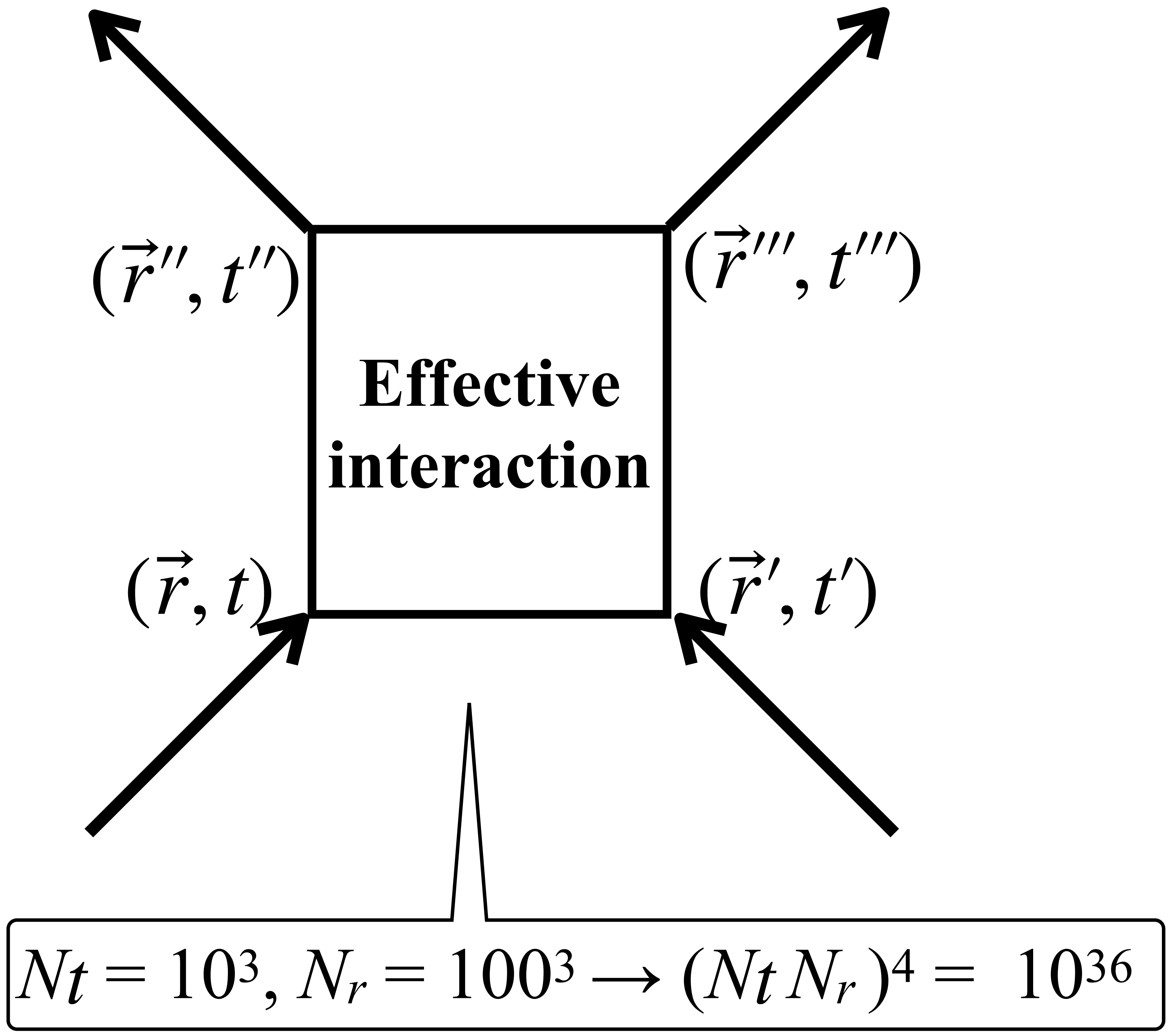
One-particle (1P) level

Symmetry breaking



Two-particle (2P) level

Susceptibility, beyond mean field



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Matsubara-frequency domain

imaginary time/Euclidean time

Required ability to handle a wide range of energy scales $> 10^4$

From band width (>100 eV) to low temperature (1K ~ 0.1 meV)

Prior knowledge $G(\tau)$ is related to $\rho(\omega)$ through ill-posed analytic continuation kernel

$$G(\tau) = \int_0^\beta \mathrm{d}\tau\ K(\tau, \omega)\rho(\omega)$$

- Intermediate representation + sparse sampling
  HS *et al.*, PRB **96**, 035147 (2017)
  J. Li *et al.*, **HS**, PRB **101**, 035144 (2020)
  HS *et al.*, SciPost Phys. Lect. Notes 63 (2022)
- Minmax method
  M. Kaltak and G. Kresse, PRB **101**, 205145 (2020)
- Discrete Lehmann Representation
  J. Kaye *et al.*, PRB **105**, 235115 (2022)

- *Ab initio* Migdal-Eliashberg calculation
  T. Wang,…, **HS**, … R. Arita, PRB **102**, 134503 (2020)
- Multi-orbital FLEX for unconventional superconductivity
  N. Witt *et al.*, PRB **103**, 205148 (2021)
- *Ab initio* self-energy embedding for transition metal oxides
  S. Iskakov *et al.*, PRB **102**, 085105 (2020)

The idea does not generalize to other domains, e.g., real-time, momentum space…

PRX **13**, 021015 (2023), arXiv:2303.11819

Other domains

Multi Matsubara domain

Overcomplete basis based on analytic continuation kernel

HS *et al*., PRB **97**, 205111 (2018), HS *et al*., SciPost Phys. **8**, 012 (2020), M. Wallerberger, HS, A. Kauch, PRR **3**, 033168 (2021), S.-S. B. Lee *et al*., PRX **11**, 041007 (2021), F. B. Kugler *et al*., PRX **11**, 041006 (2021)

Computation on the overcomplete basis is cumbersome.

Real-time (non-equilibrium) domain

Hierarchical low-rank compression J. Kaye, Denis Golež, SciPost Phys. **10**, 091 (2021)

Multi momentum domain

Truncated form-factor basis C. J. Eckhardt *et al*., PRB **98**, 075143 (2018), C. J. Eckhardt *et al*., PRB **101**, 155104 (2020)

General compact bases are still under active development.

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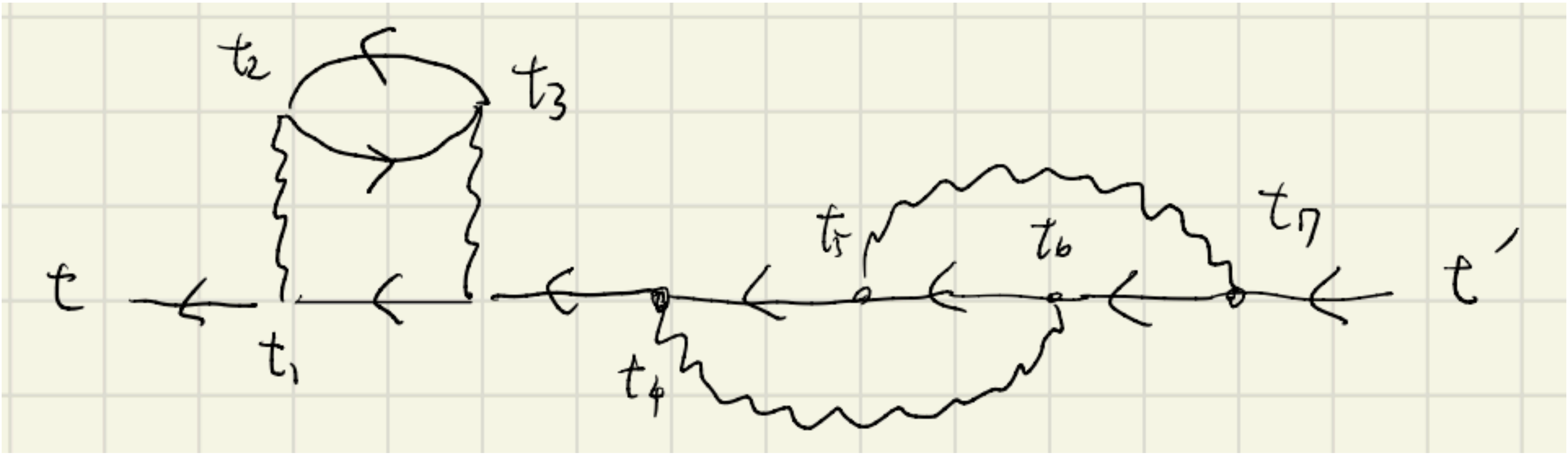
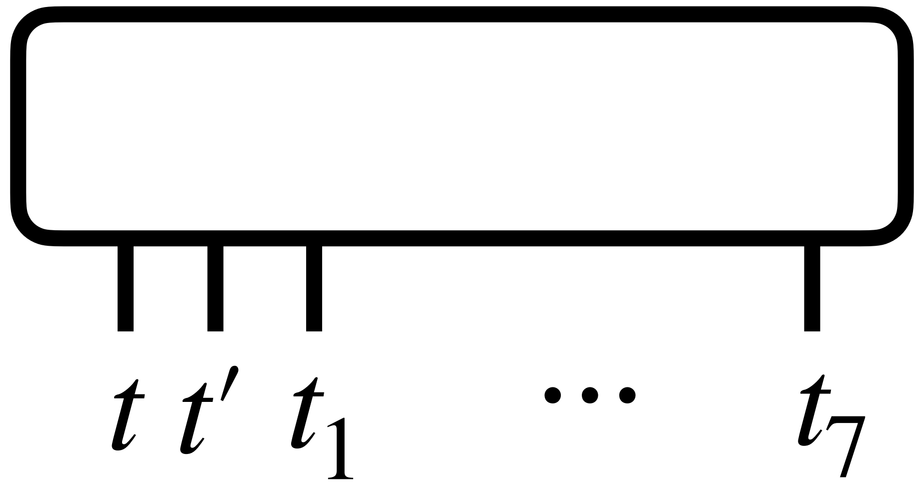
Feynman diagram/correlation function is tensor



$$= \int dt_1 \cdots dt_7 \; F(t, t'; t_1, \cdots, t_7) = G(t, t')$$



Any *compact* tensor network representation?

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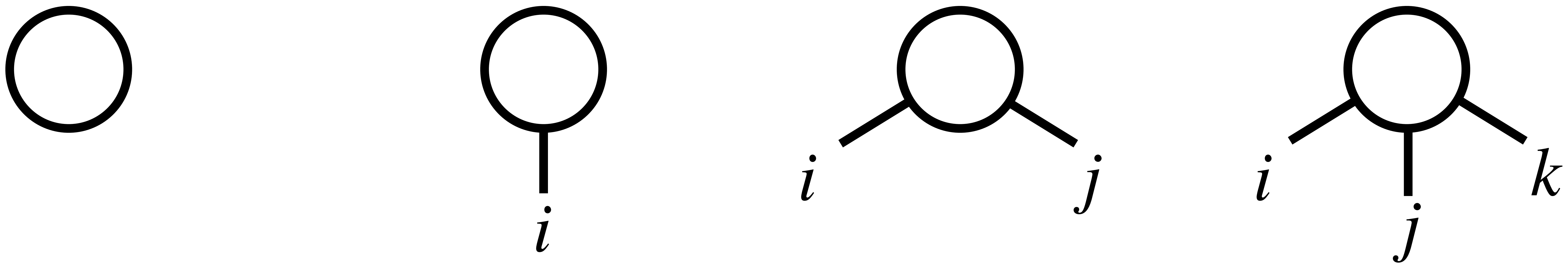
Warm-up: Tensor diagram notation

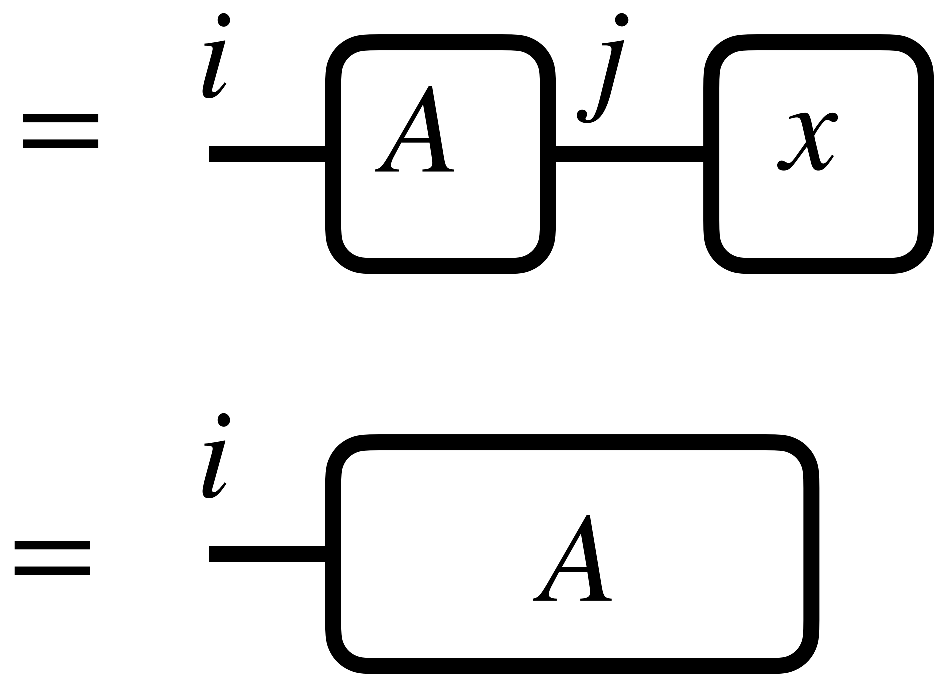
Scalar	Vector	Matrix	Three-way tensor
a	a_i	a_{ij}	a_{ijk}



A leg sticking out corresponds to an index.

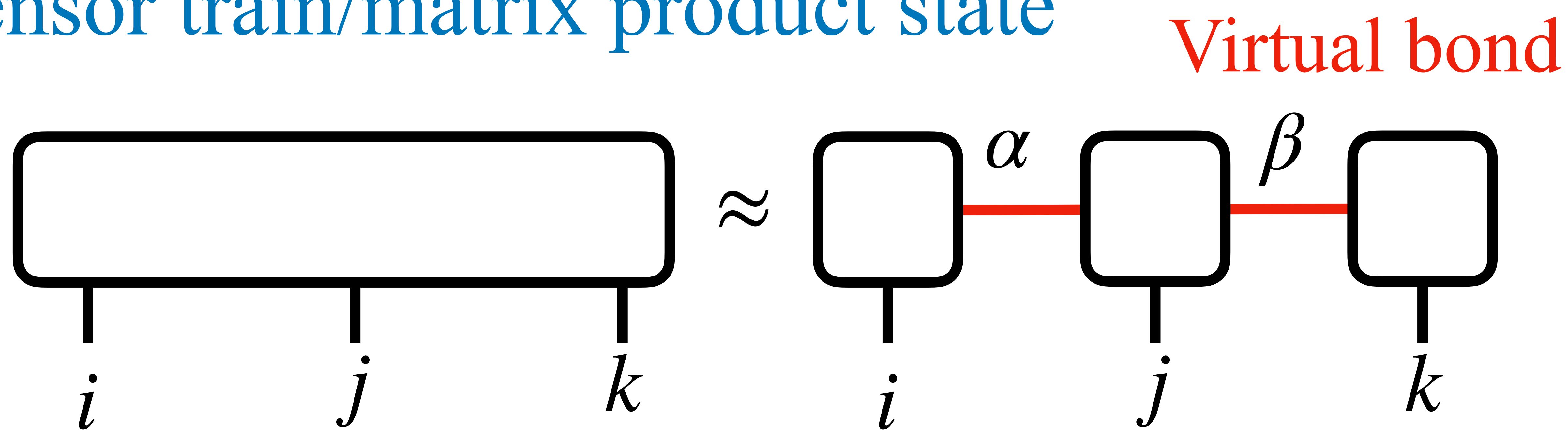
Contraction

$$\sum_j A_{ij} x_j =$$



Summation over shared indices

Tensor train/matrix product state



Compression for small bond dimensions!
Singular value decomposition, cross interpolation…

https://tensornetwork.org/diagrams/
PRX **13**, 021015 (2023), arXiv:2303.11819

Previous study: Learning Feynman diagram

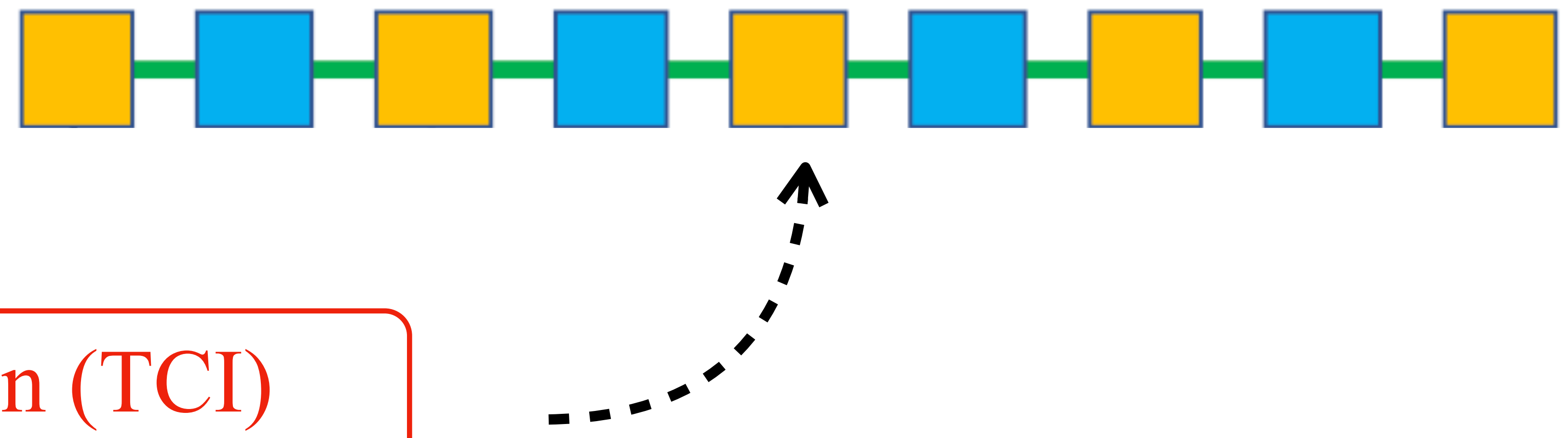
Y. N. Fernández *et al.*, PRX **12**, 041018 (2022)

Weak-coupling expansion in real time

$H = H_0 + UH_{\mathrm{int}}$ $\quad Q(U) = \sum_n Q_n U^n$ Charge, Green's function, *etc*.

Single-orbital Anderson impurity model

$$Q_n = \int dv_1 \ldots dv_n \tilde{Q}_n(v_1, \ldots, , v_n),$$

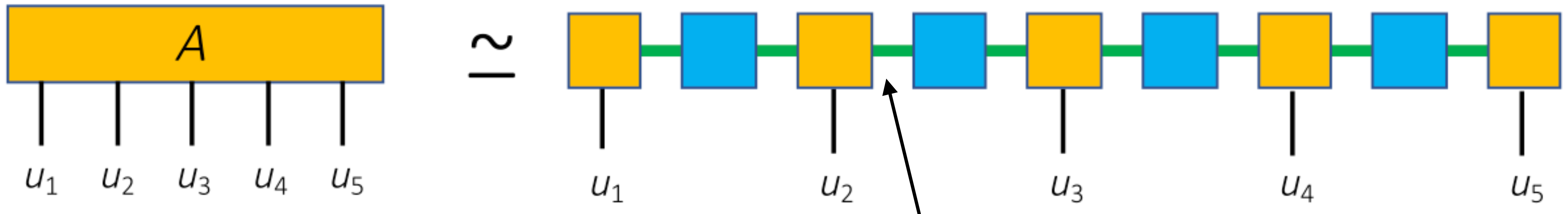


Low-rank approximation by Tensor Cross Interpolation (TCI)

$$\tilde{Q}_n(v_1, \ldots, v_n) \approx M_1(v_1) \cdots M_n(v_n),$$

$$Q_n \approx \left(\int dv_1 M_1(v_1)\right) \cdots \left(\int dv_n M_n(v_n)\right)$$

TCI



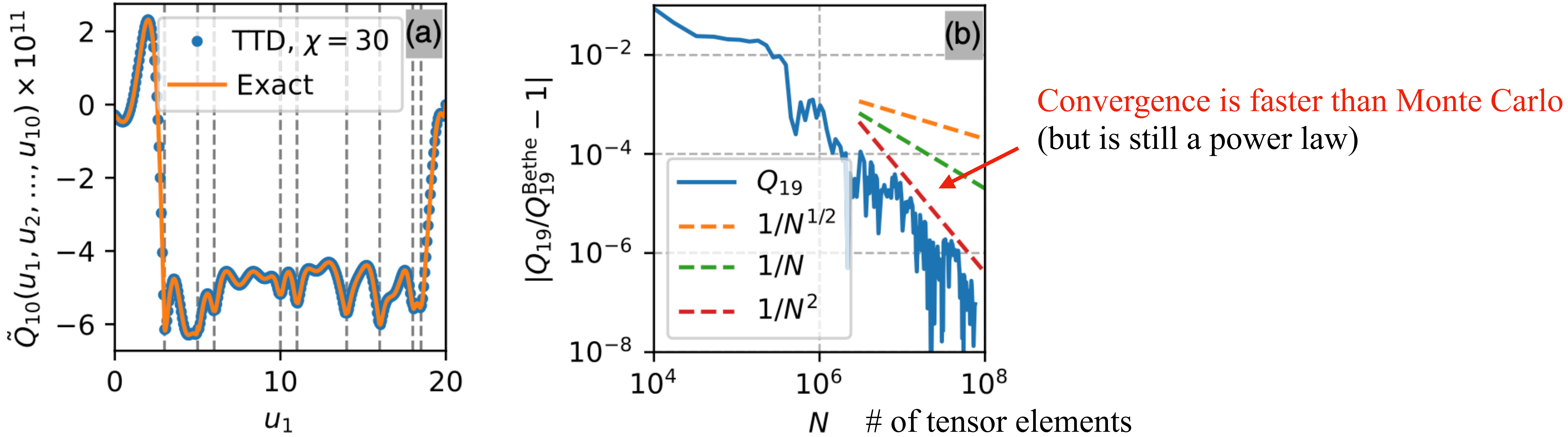
Non-trivial: Bond dimensions are small?

PRX **13**, 021015 (2023), arXiv:2303.11819

Previous study: Learning Feynman diagram

Y. N. Fernández *et al.*, PRX **12**, 041018 (2022)

19th order diagram



Sign problem free, replacement for quantum Monte Carlo
(in some cases)

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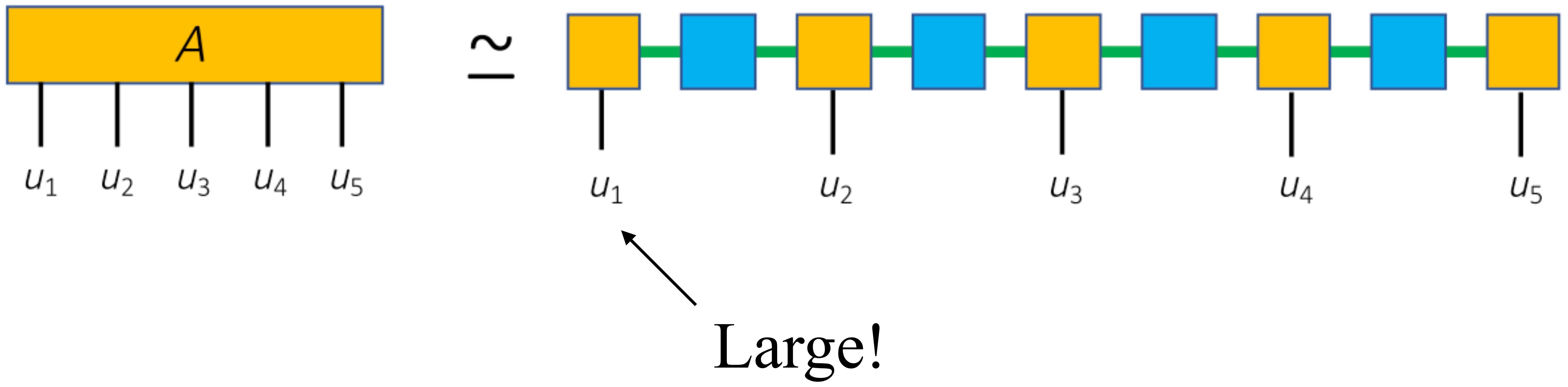
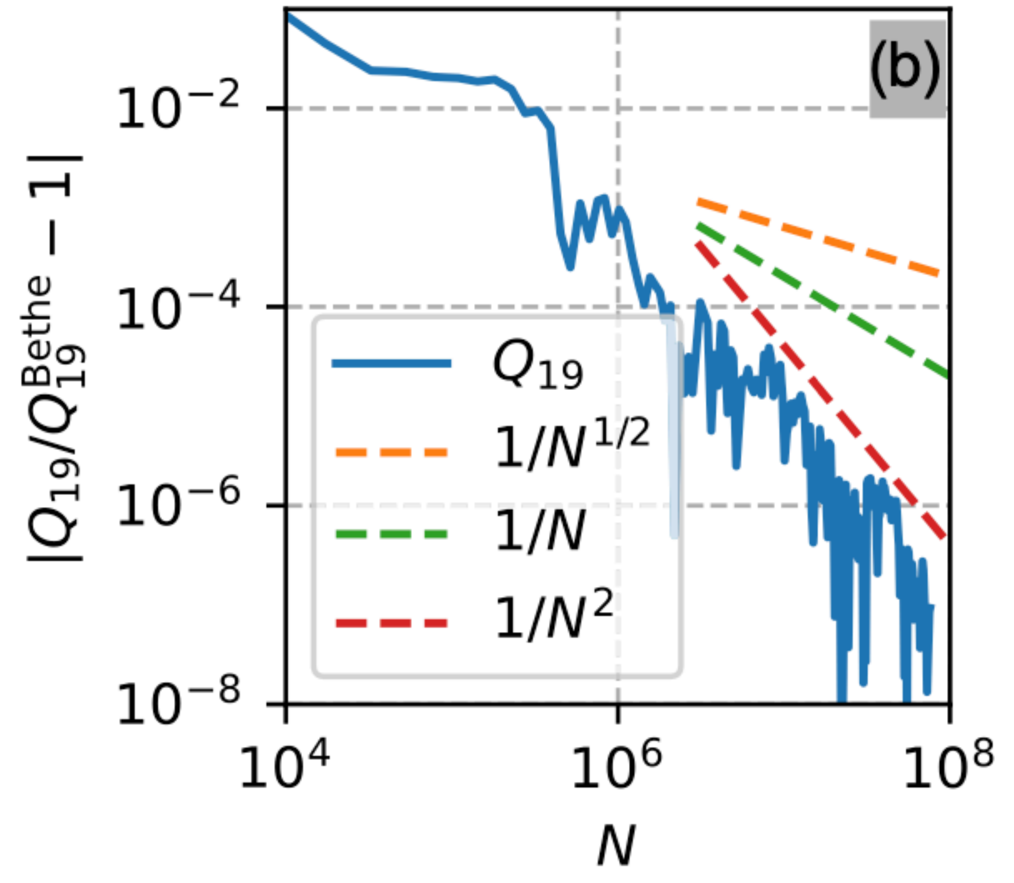
Remaining issues



- How to treat a wide range of coexisting length scales?
- Can we achieve exponential convergence?
- Computation (convolution, Fourier transform…)



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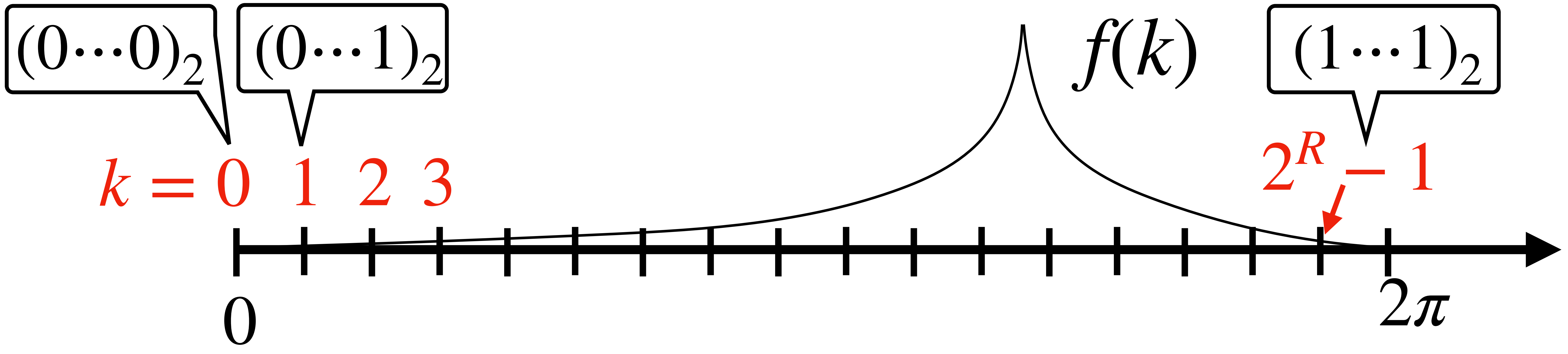
- Outlook & summary

Quantics tensor train (QTT)

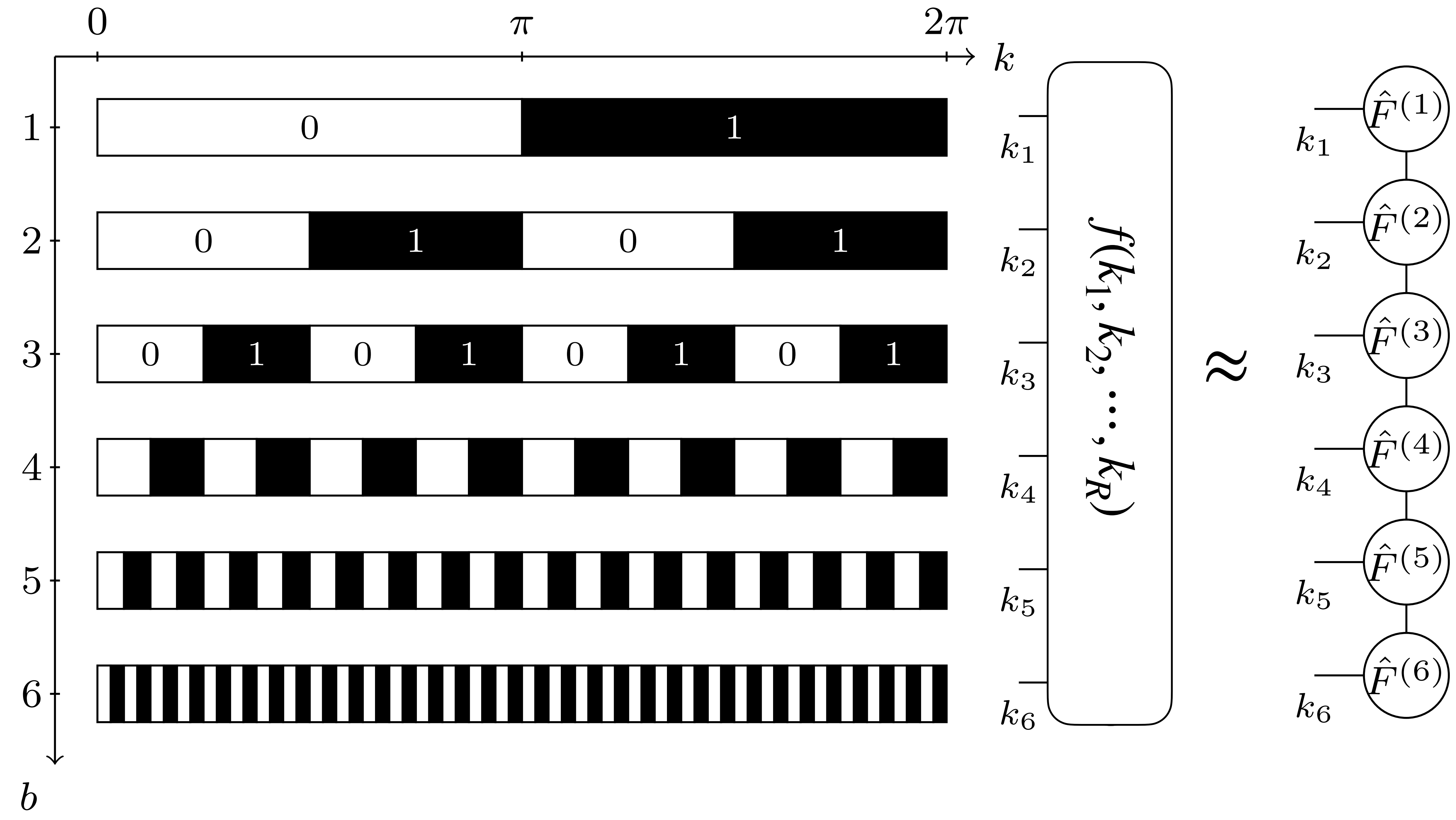
I. V. Oseledets, Doklady Math. **80**, 653 (2009)

B. N. Khoromskij, Constr. Approx. **34**, 257 (2011)

For image compression José I. Latorre, arXiv:quant-ph/0510031v1



$k = (k_1 \cdots k_{R-1} k_R)_2$



Length-scale separation → Bond dimension $\ll 2^{R/2}$

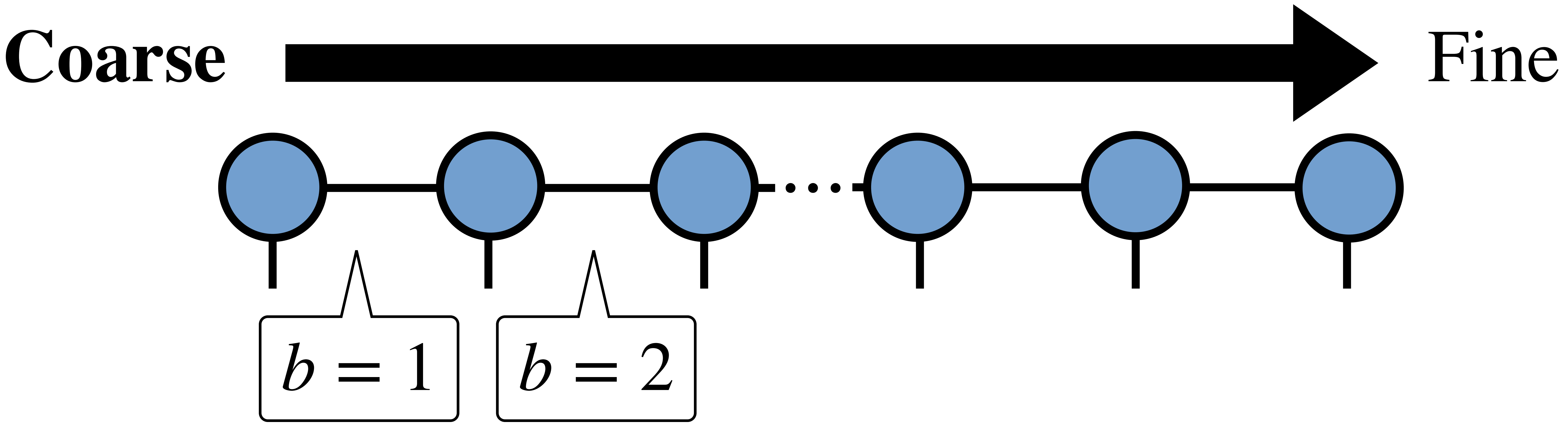
$$f(k_1, k_2, \cdots, k_R) \approx \sum_{\alpha_1=1}^{D_1} \cdots \sum_{\alpha_{R-1}=1}^{D_{R-1}} \hat{F}^{(1)}_{k_1,1\alpha_1} \hat{F}^{(2)}_{k_1,\alpha_1\alpha_2} \cdots \hat{F}^{(R)}_{k_R,\alpha_{R-1}1}$$

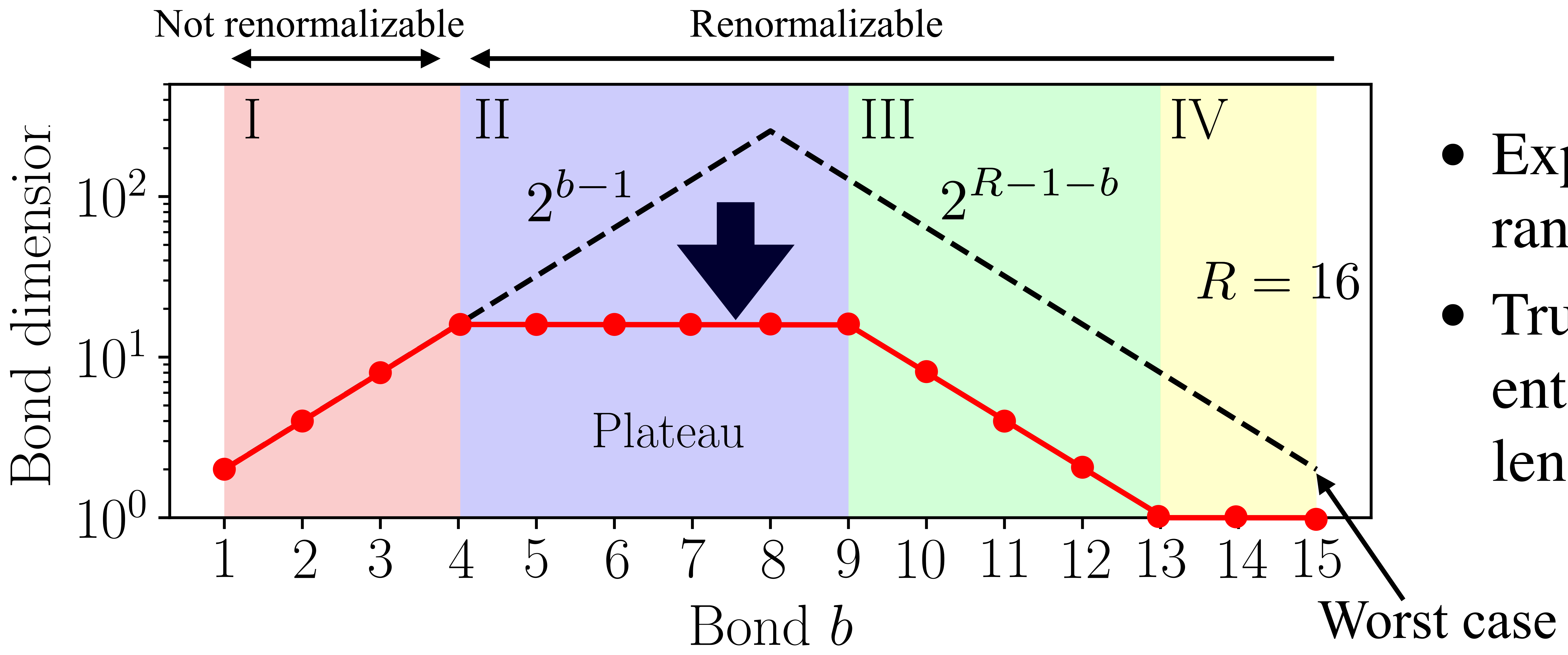
Tensor train/Matrix product state

QTT can represent a low-entanglement structure between different length scales!

PRX **13**, 021015 (2023), arXiv:2303.11819

Length-scale separation





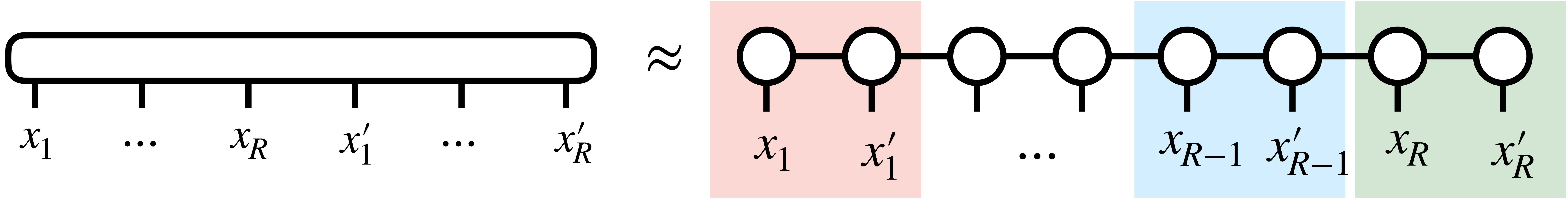
- Exponentially wide range of length scales
- Truncation limits entanglement between length scales.

PRX **13**, 021015 (2023), arXiv:2303.11819

Multivariate functions

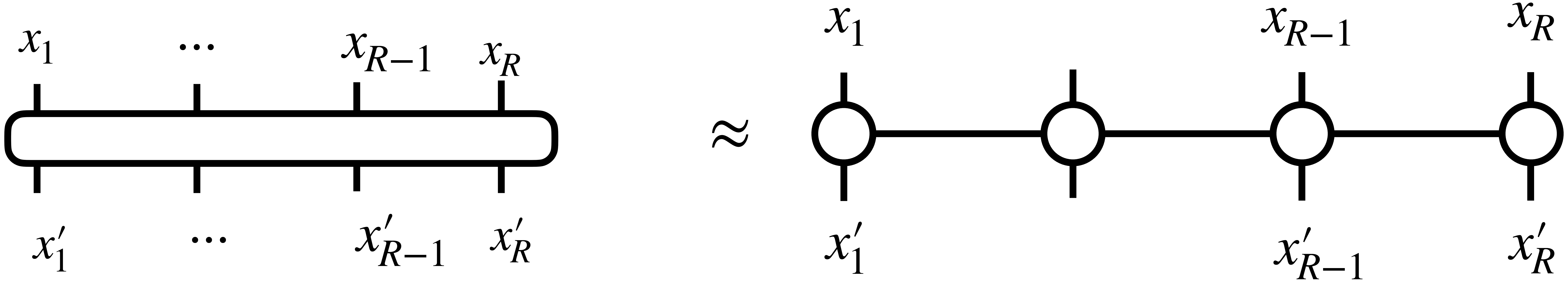
Same length scale

$f(x, x')$



$x = (0.x_1x_2 \cdots x_n \cdots)_2 \in [0,1)$

$x' = (0.x'_1x'_2 \cdots x'_n \cdots)_2 \in [0,1)$



"Matrix product operator" (MPO)

PRX **13**, 021015 (2023), arXiv:2303.11819

Function with trivial QTT representation

Exponential $f(x) = e^{-x} = e^{-x_1/2} e^{-x_2/2^2} \cdots e^{-x_n/2^n} \cdots$ $\quad D = 1$

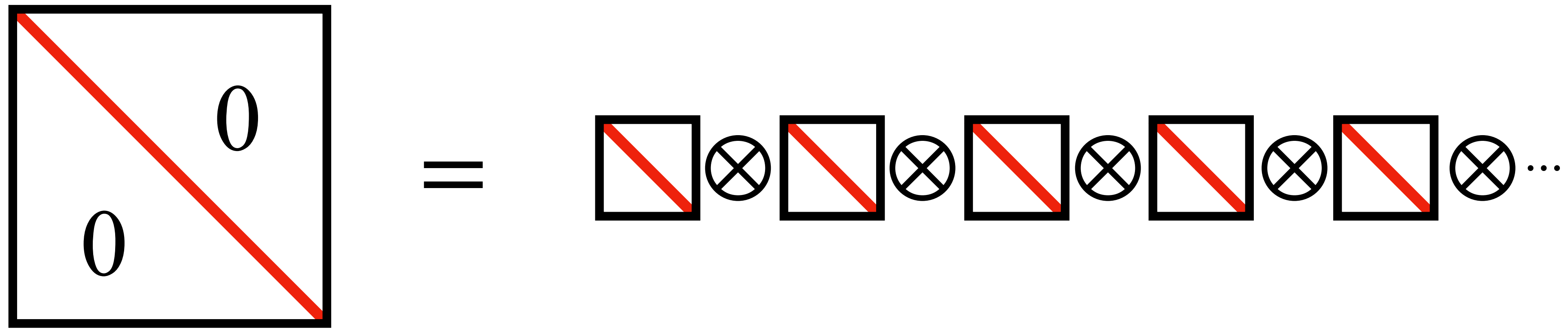
$$x = (0.x_1 x_2 \cdots x_n \cdots)_2 \in [0,1)$$

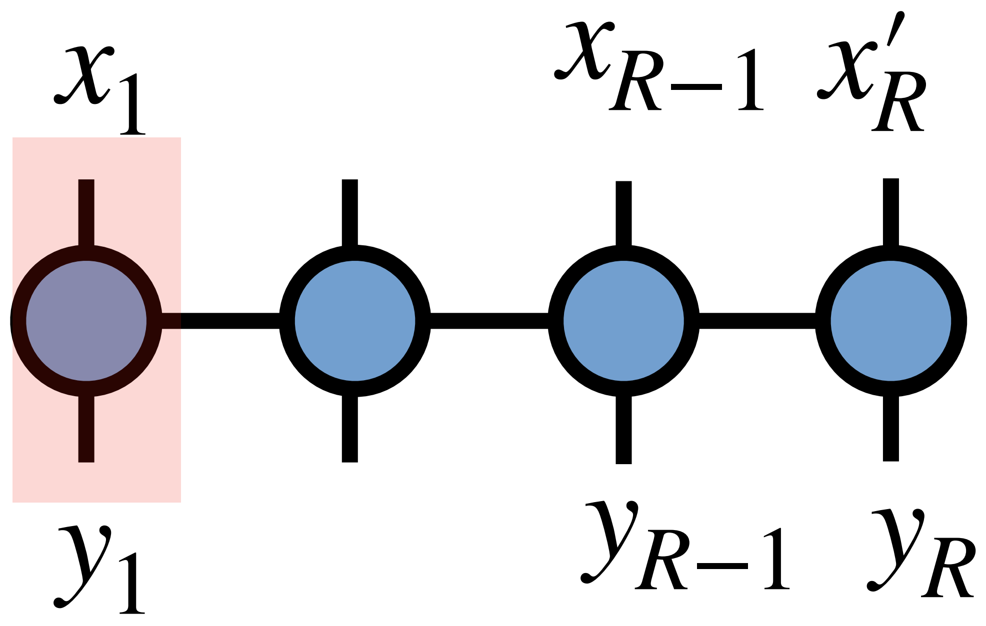
The Sum of N exponential functions can be represented as a QTT of rank at most N.
∵ Bond dimensions are added when MPSs are added.

Polynomial $D \leq 1 + p$

M. Ali and A. Nouy, "A. Approximation Theory of Tree Tensor Networks: Tensorized Univariate Functions", Constr Approx (2023)

Identity matrix $f(x, y) = \delta_{x,y} = \delta_{x_1,y_1} \delta_{x_2,y_2} \cdots$ $\quad D = 1$





Representation of Continuous Functions: https://tensornetwork.org/functions/

Written by Miles Stoudenmire

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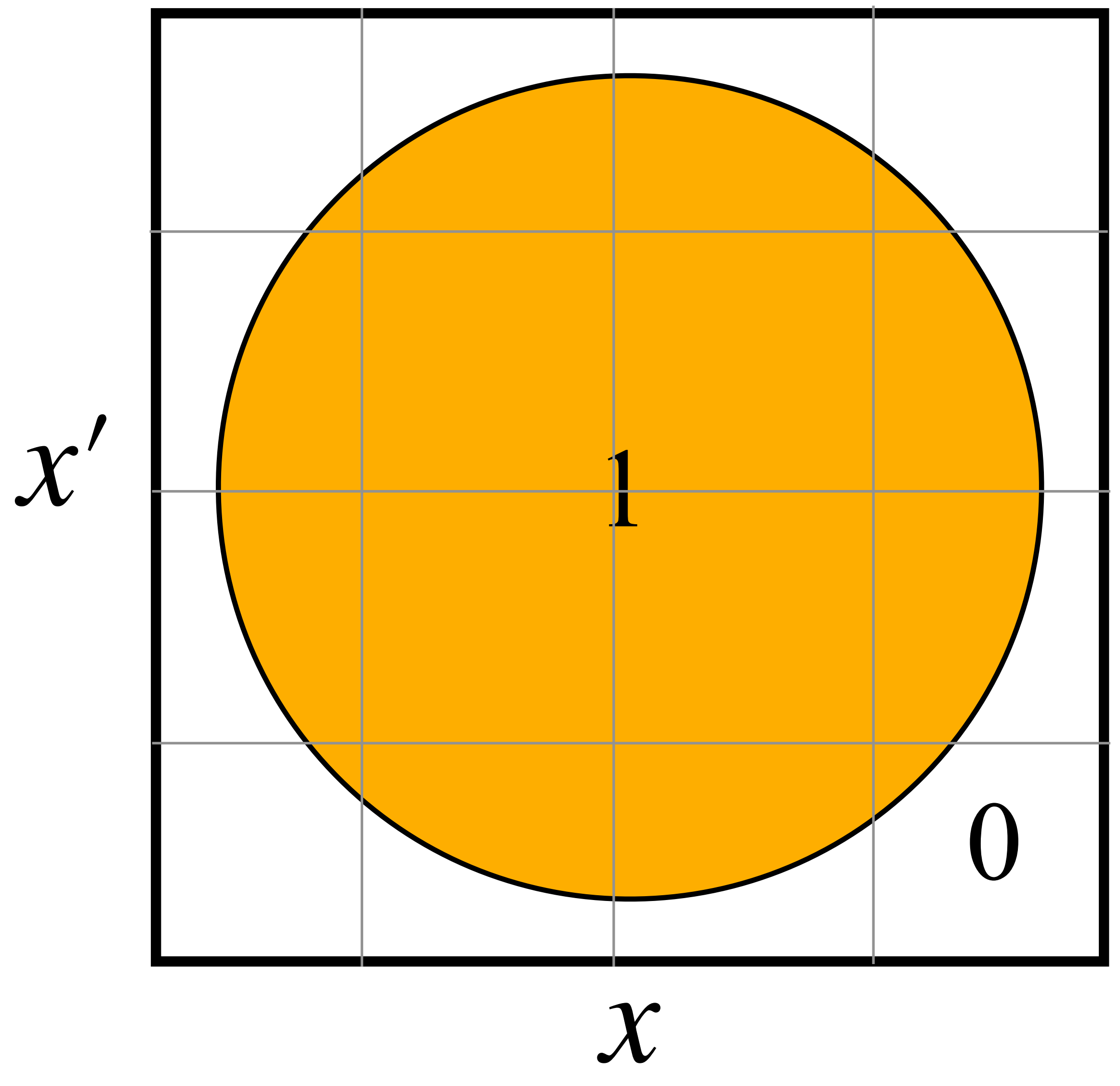
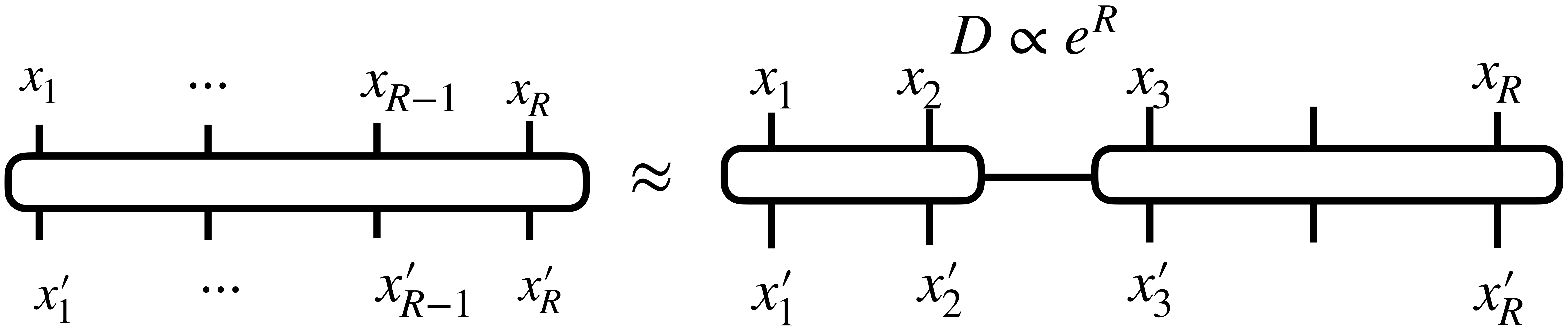
Non-compressible multivariate functions



Many linearly independent patches



Singular value decomposition

My naive understanding

Step functions with gradually changing angles are not compressible.

Broadening and/or the fixed number of angles may help.

Line discontinuity→OK

or, in other words, if A is partitioned into $2^k \times 2^k$ blocks B_{pq}, $p, q = 1, \ldots, 2^{d-k}$, then r_k is equal to the dimension of linear space spanned by matrices B_{pq}.

For this example, it is easy to see that each splitting into $2^k \times 2^k$ blocks produces $\mathcal{O}(n)$ different linearly independent blocks. Therefore

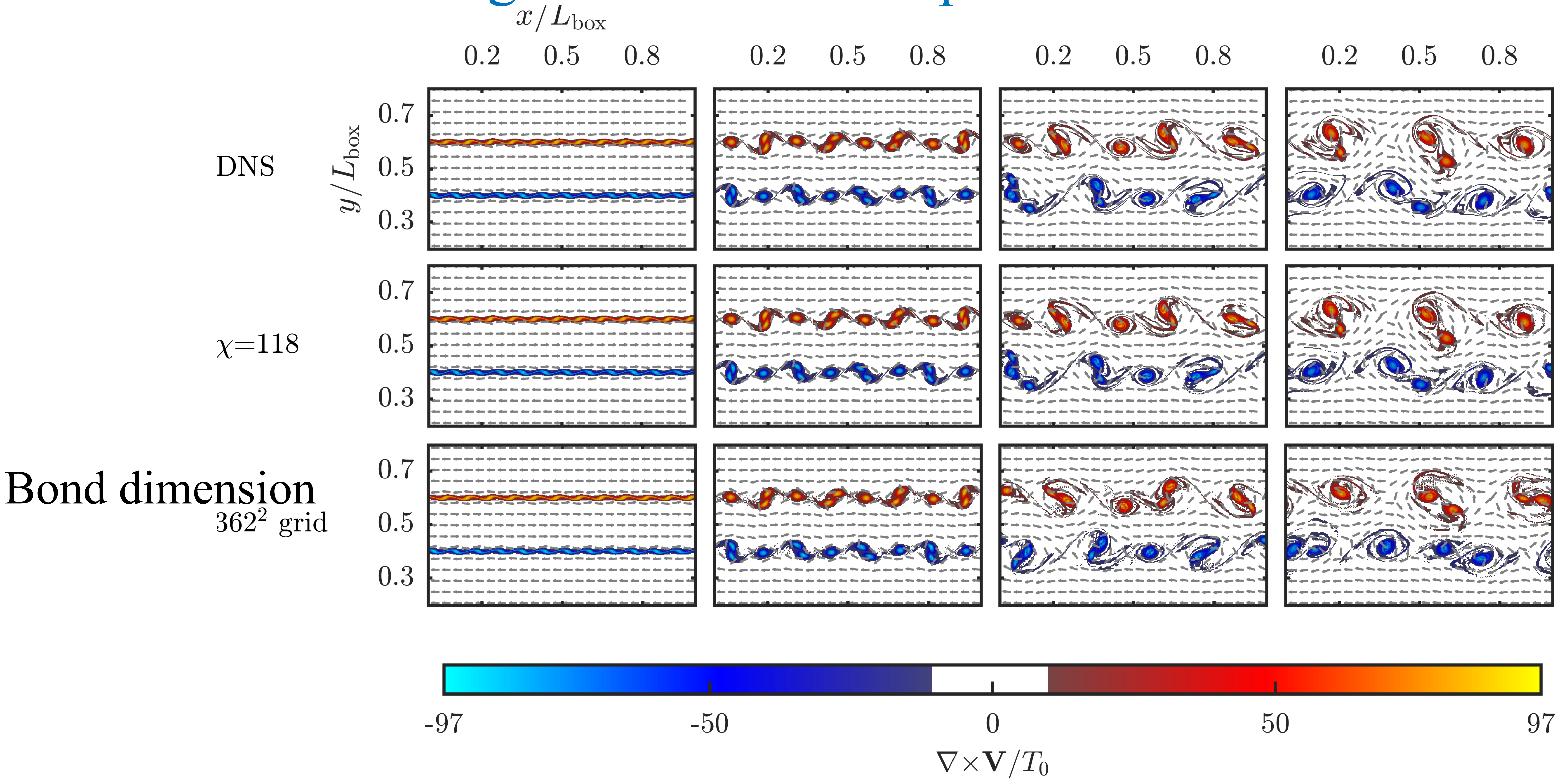
$$r_k = \mathcal{O}(n),$$

and the memory to store matrices $U_1, \ldots, U_d$ in this case is $\mathcal{O}(n^2)$; thus no compression is provided for this simple example. However, the WTT transform with limited maximal ranks works well. For this example, there is a natural accuracy level related to discrete representation of a circle on a rectangular grid, roughly $\frac{1}{n}$, and that is confirmed by experiment. If the threshold parameter ε is set to 10^{-2}, the number of

I. V. Oseledets and E. E. Tyrtyshnikov, SIAM J. Sci. Comput. **33**, 1315 (2011)

Recent applications of QTT in physics

Solving Navier-Stokes equations for turbulent flows



N. Gourianov *et al*., Nat. Comput. Sci. **2**, 30 (2022)

Vlasov-Poisson equations for collisionless plasmas

E. Ye and N. F. G. Loureiro, arXiv:2205.11990

This study: Are correlation functions of quantum systems compressible?

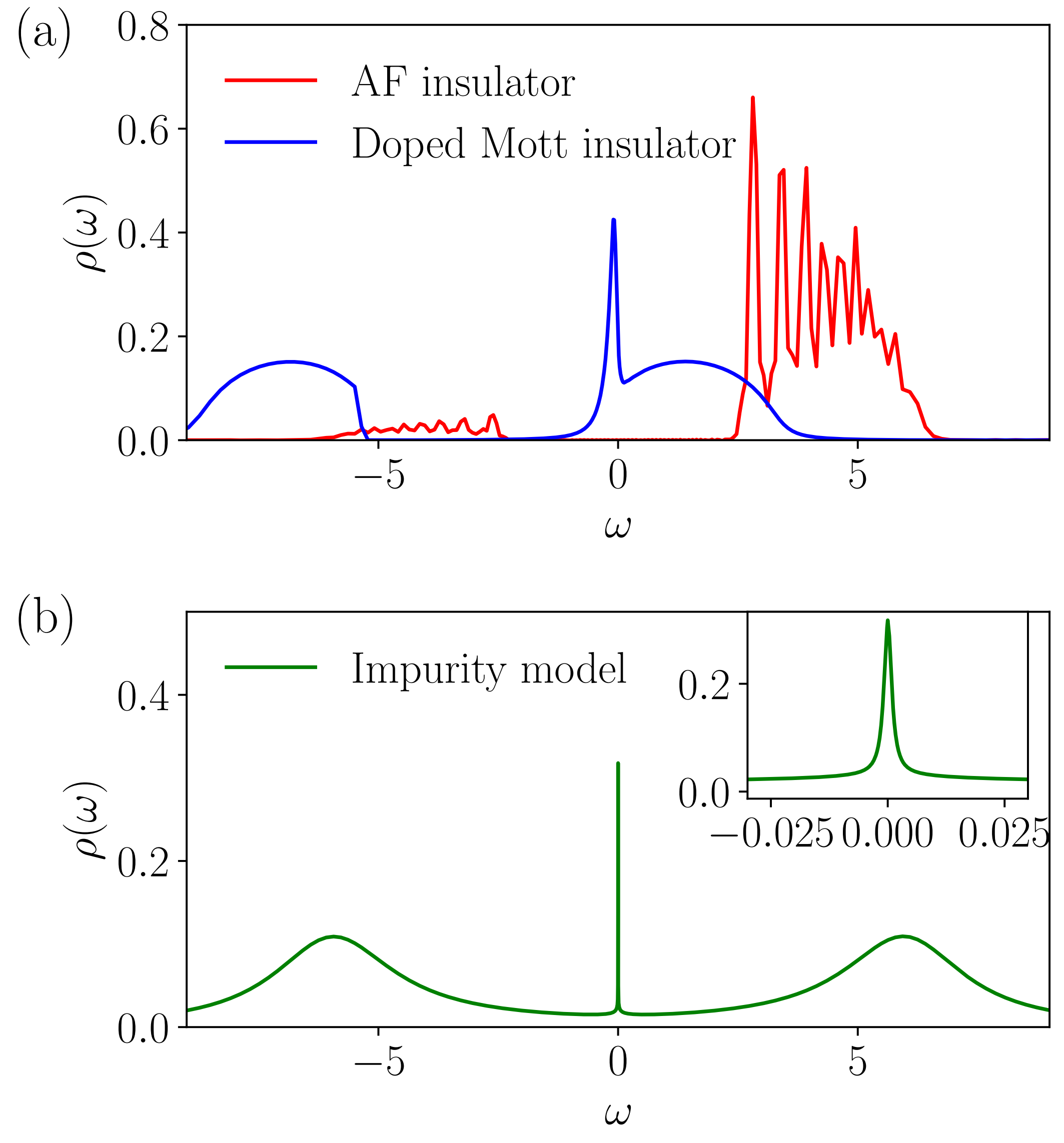
PRX **13**, 021015 (2023), arXiv:2303.11819

Compression

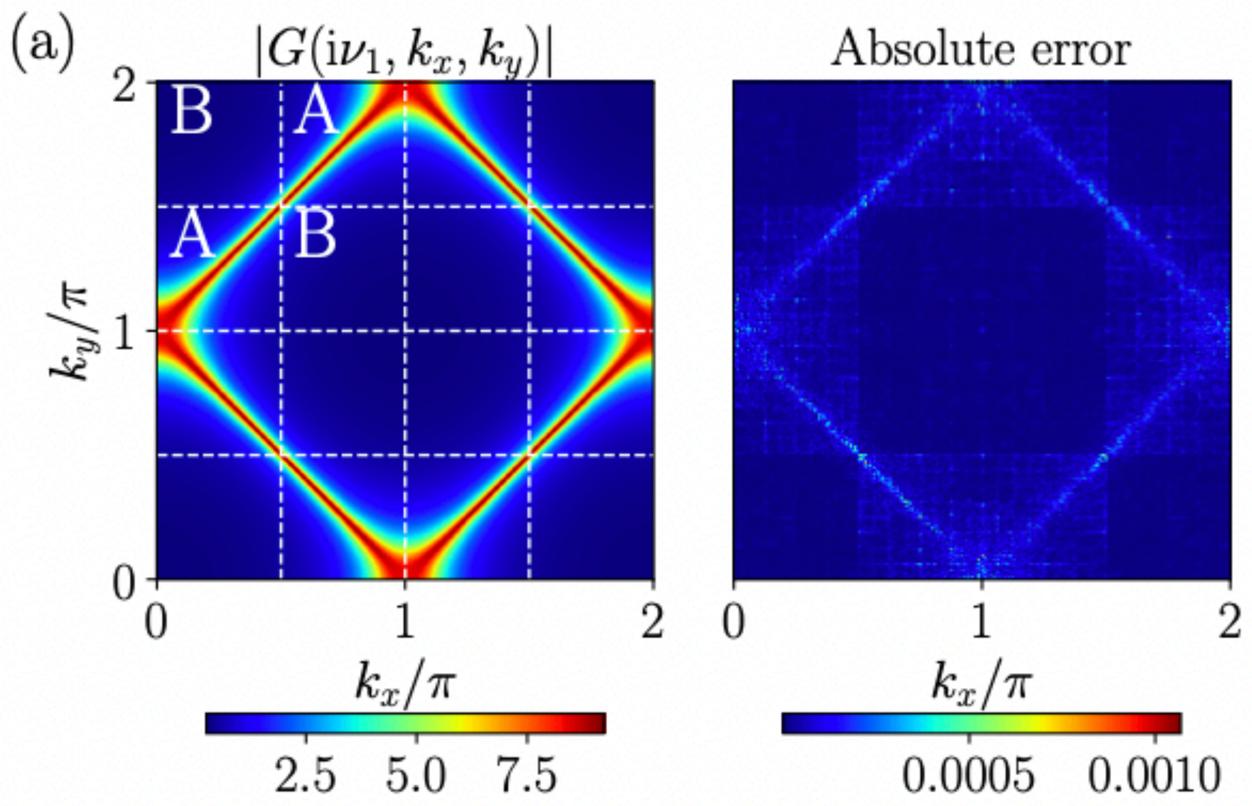
PRX **13**, 021015 (2023), arXiv:2303.11819

Compression

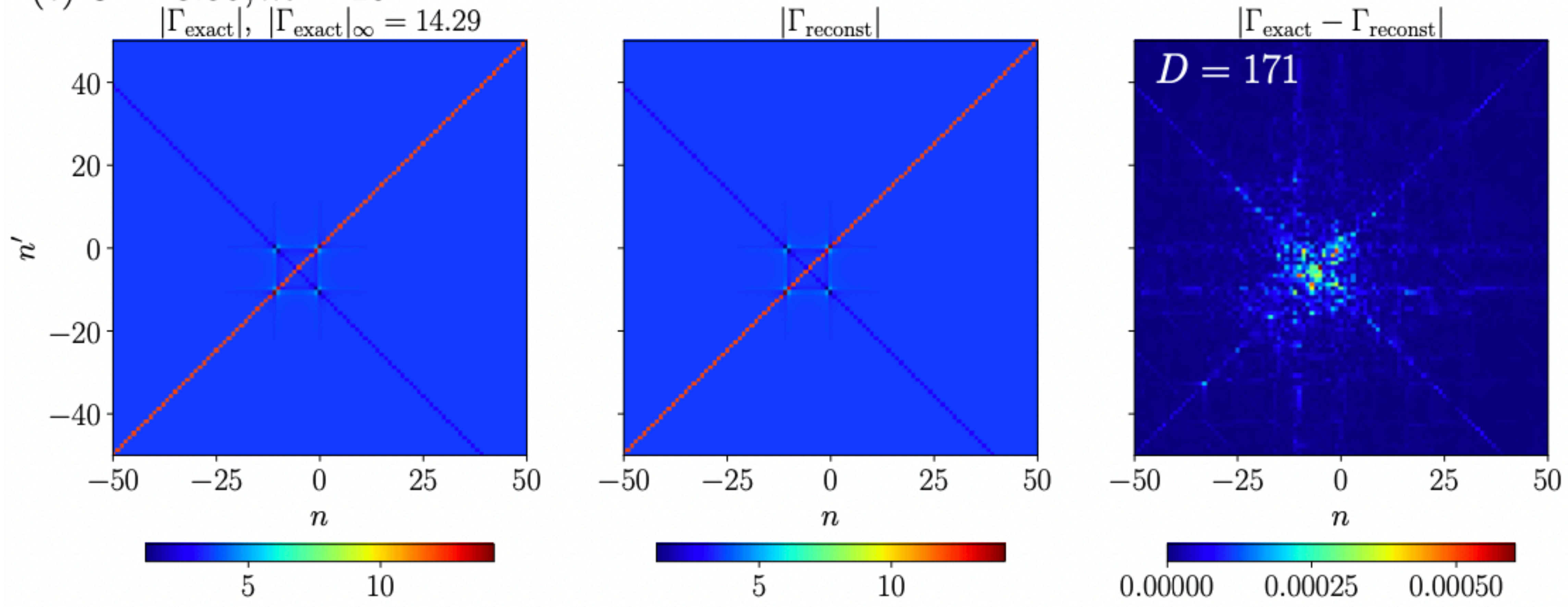
Spectral function



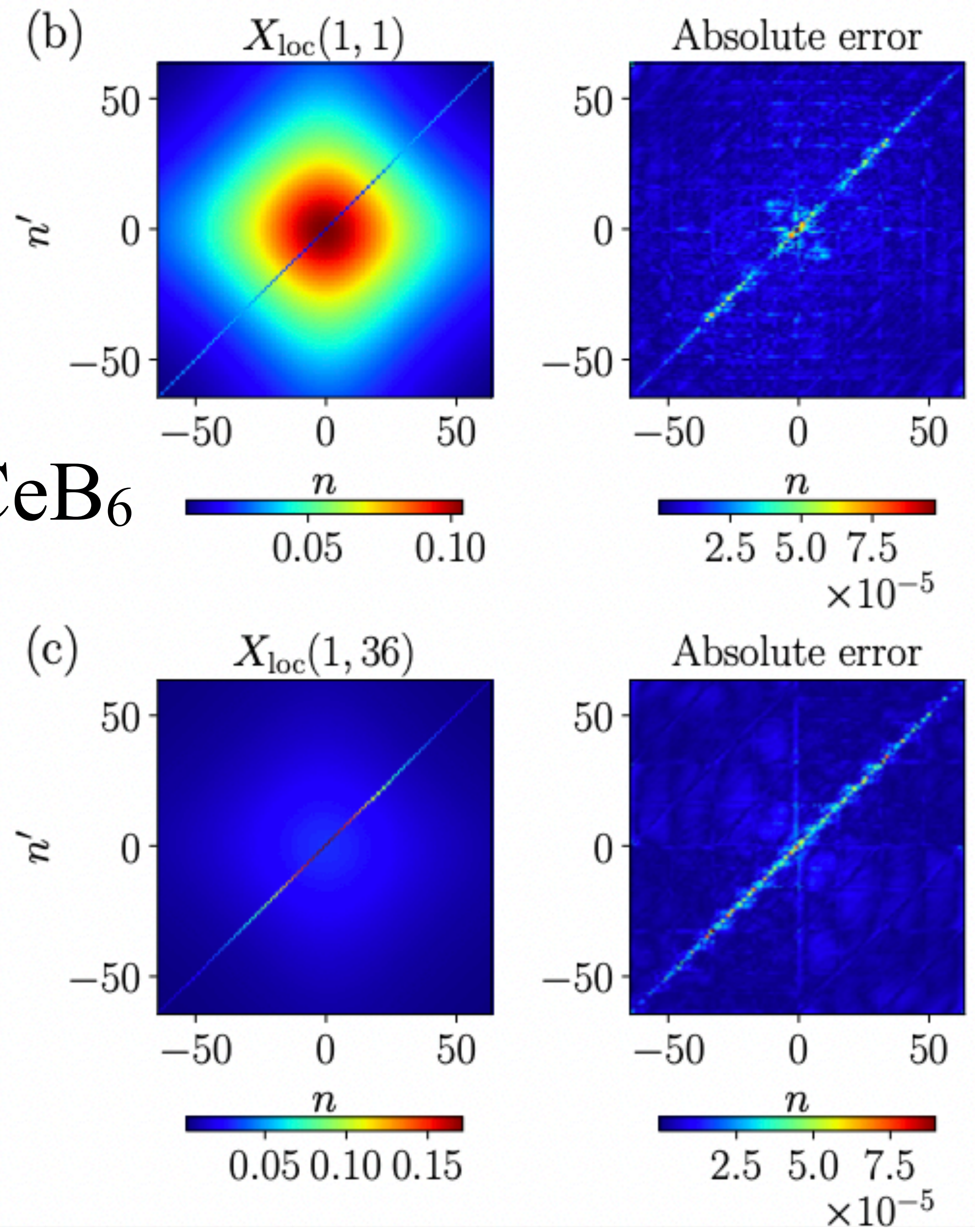
1P momentum space



2P vertex functions



Multipolar susceptibility

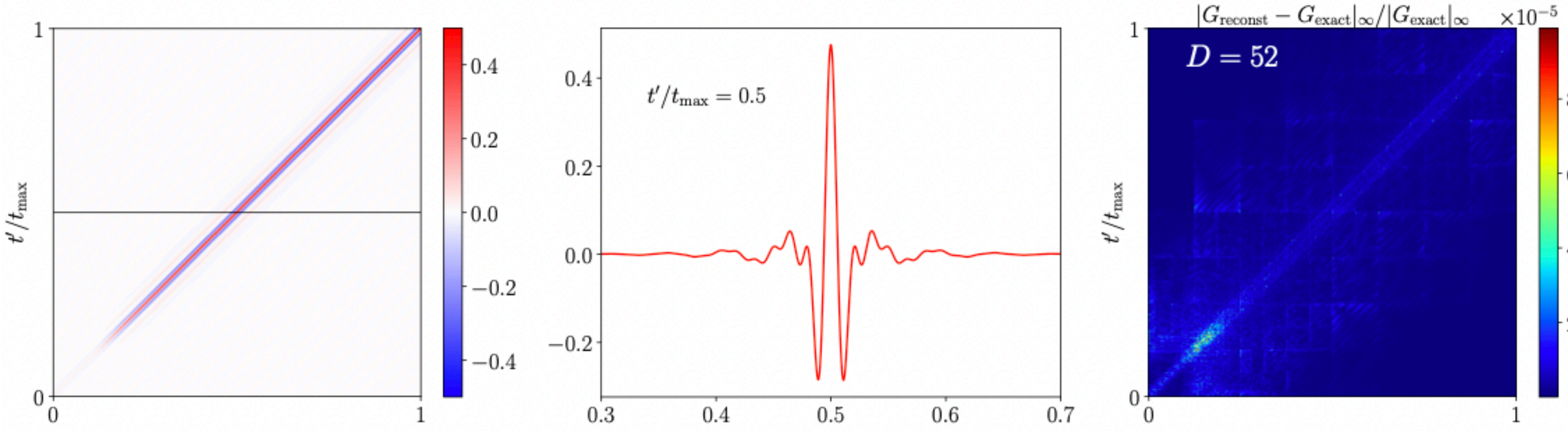


CeB$_6$

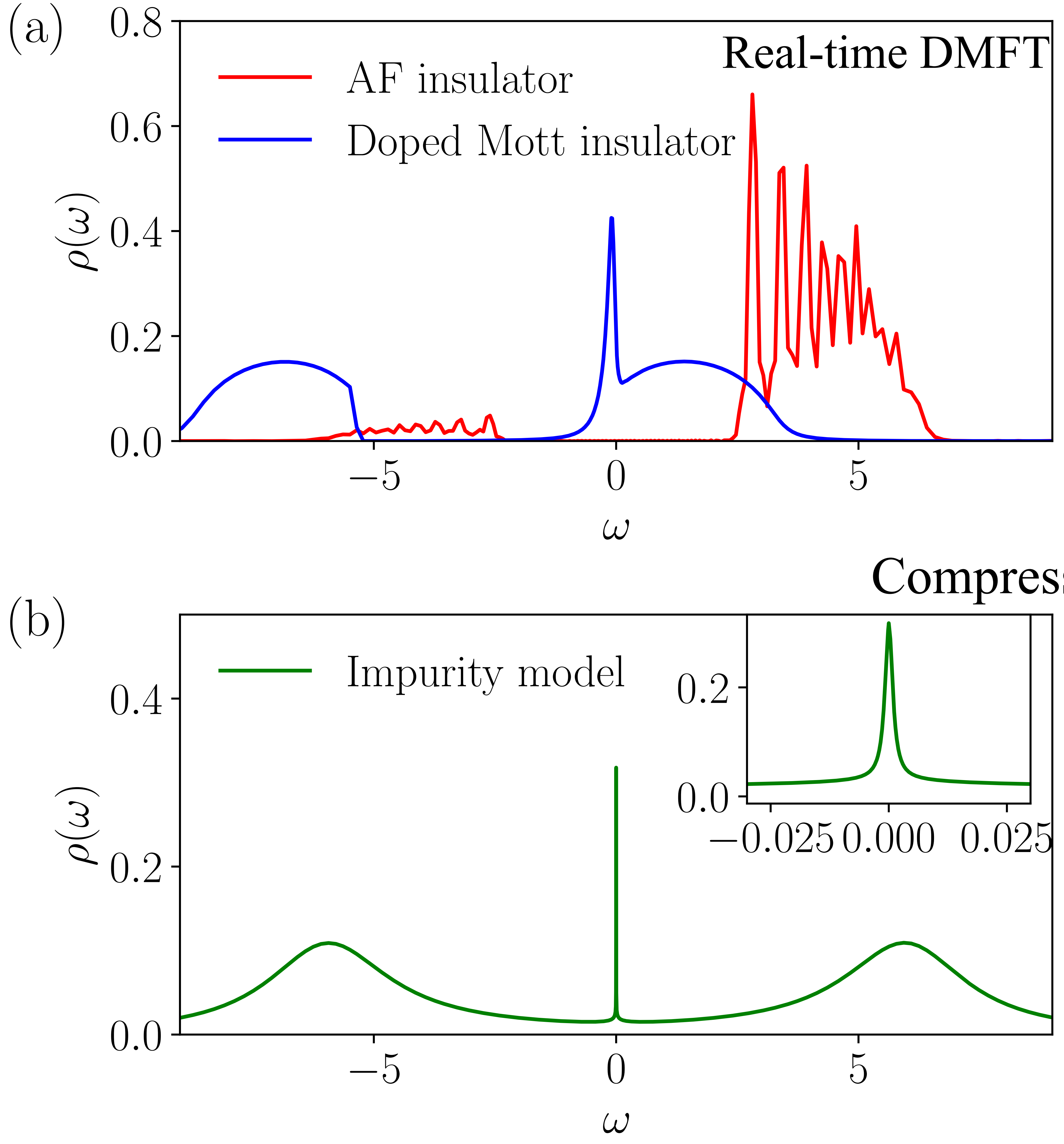
All QTT compressible!

HS *et al*., PRX **13**, 021015 (2023)

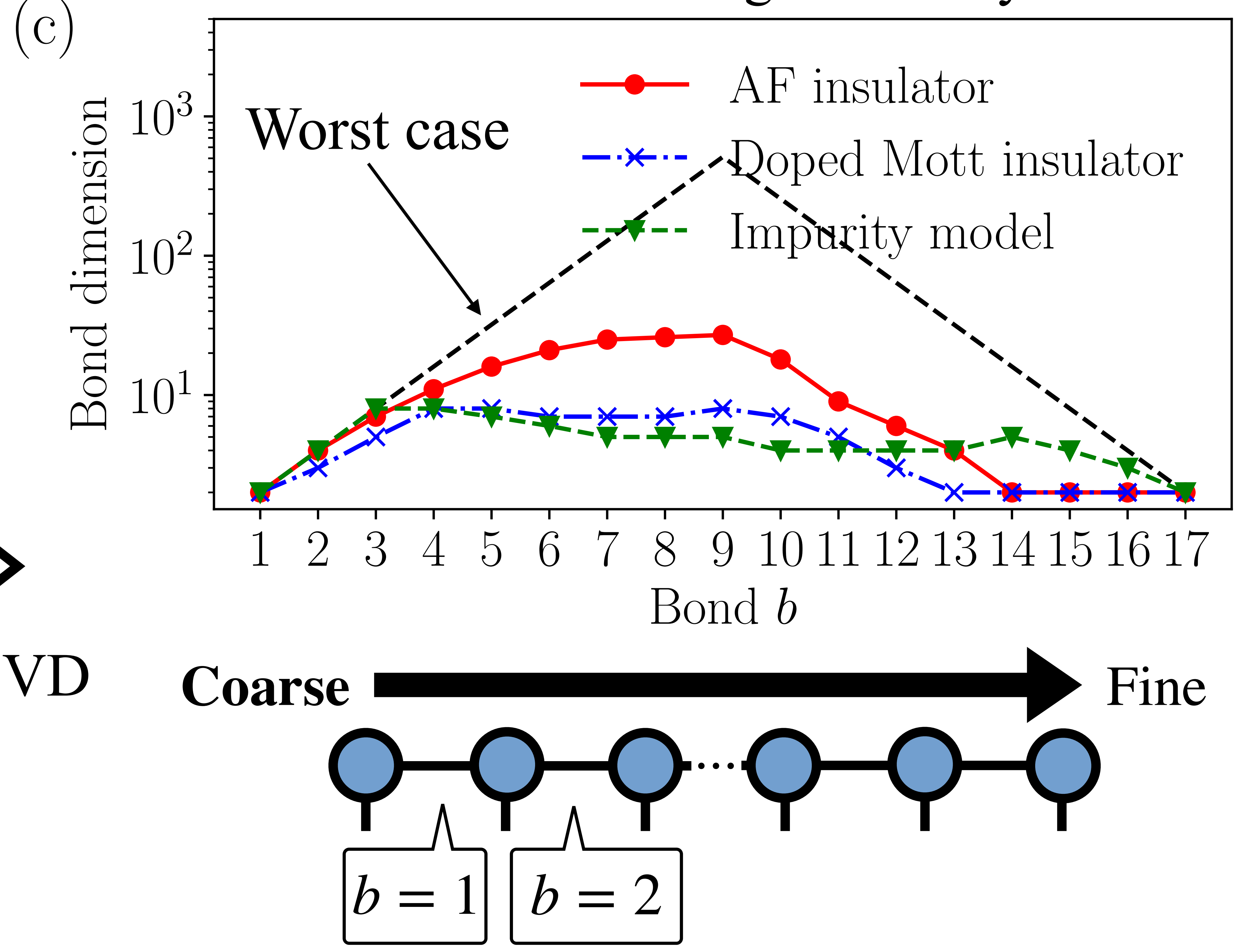
Nonequilibrium system (real-time Green's function)



Spectral functions



Compression by SVD

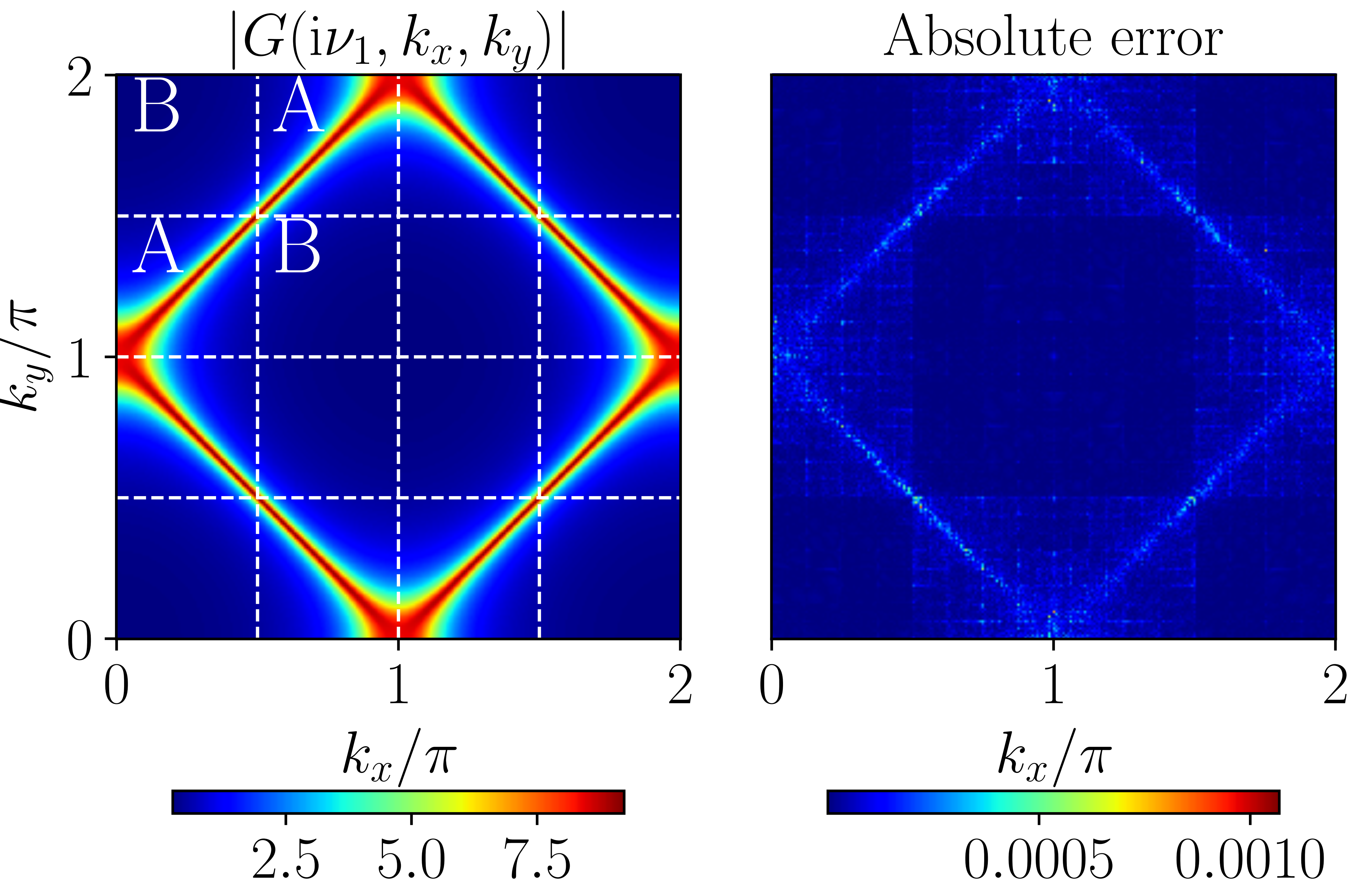


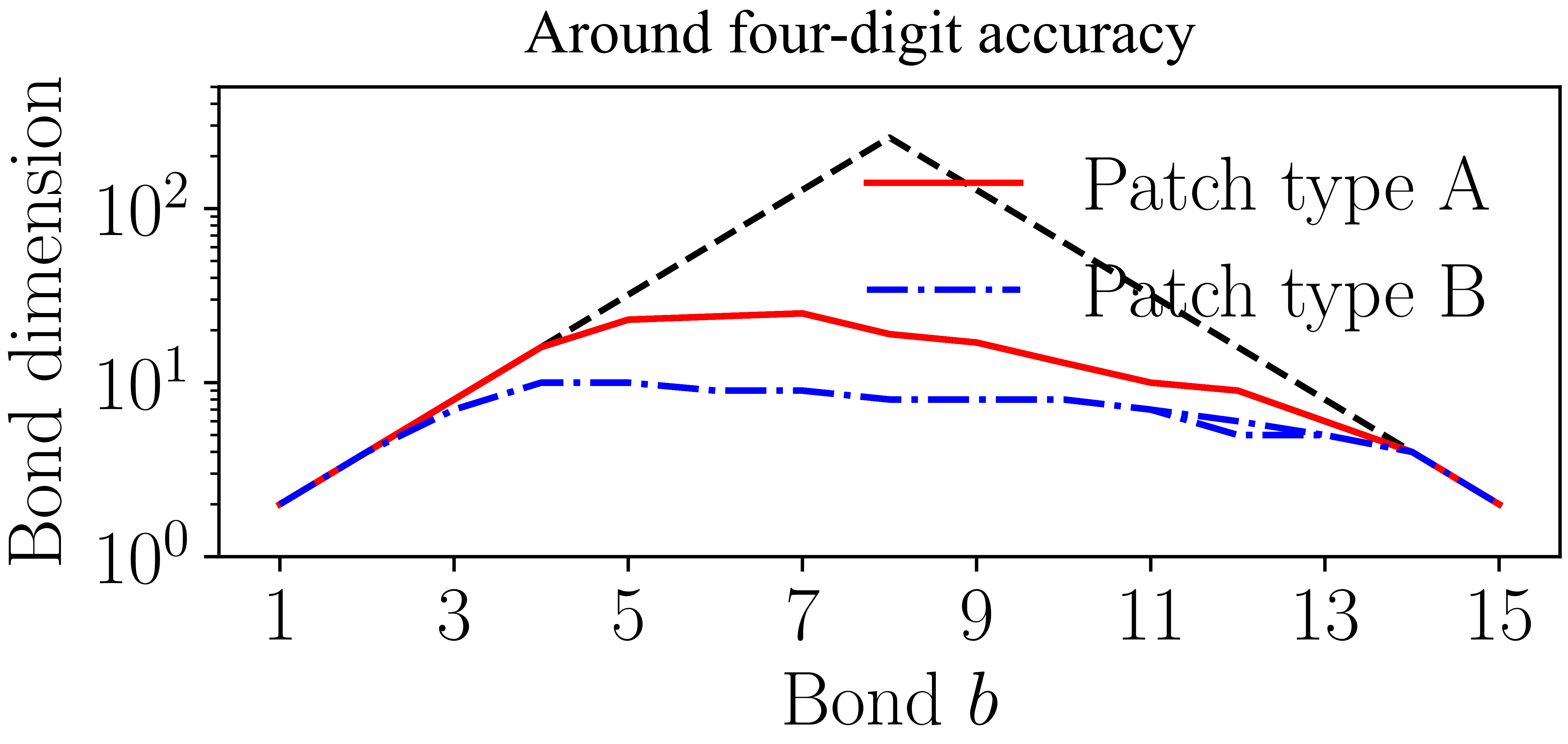
- Sharp peaks can be represented.
- Larger bond dimension for more features

PRX **13**, 021015 (2023), arXiv:2303.11819

Momentum-resolved Green's function

Hubbard model, $T = 0.03,\ U = 1.1$ (band width: 8), FLEX approximation





Our conjecture: $D \propto \beta^{\frac{d-1}{2}}$ (d: spatial dimension) $\beta = 1/T$

M. K. Ritter, Y. N. Fernández, M. Wallerberger, J. von Delft, HS, X. Waintal, arXiv:2303.11819

PRX **13**, 021015 (2023), arXiv:2303.11819

Real-time Green's function: Non-equilibrium case

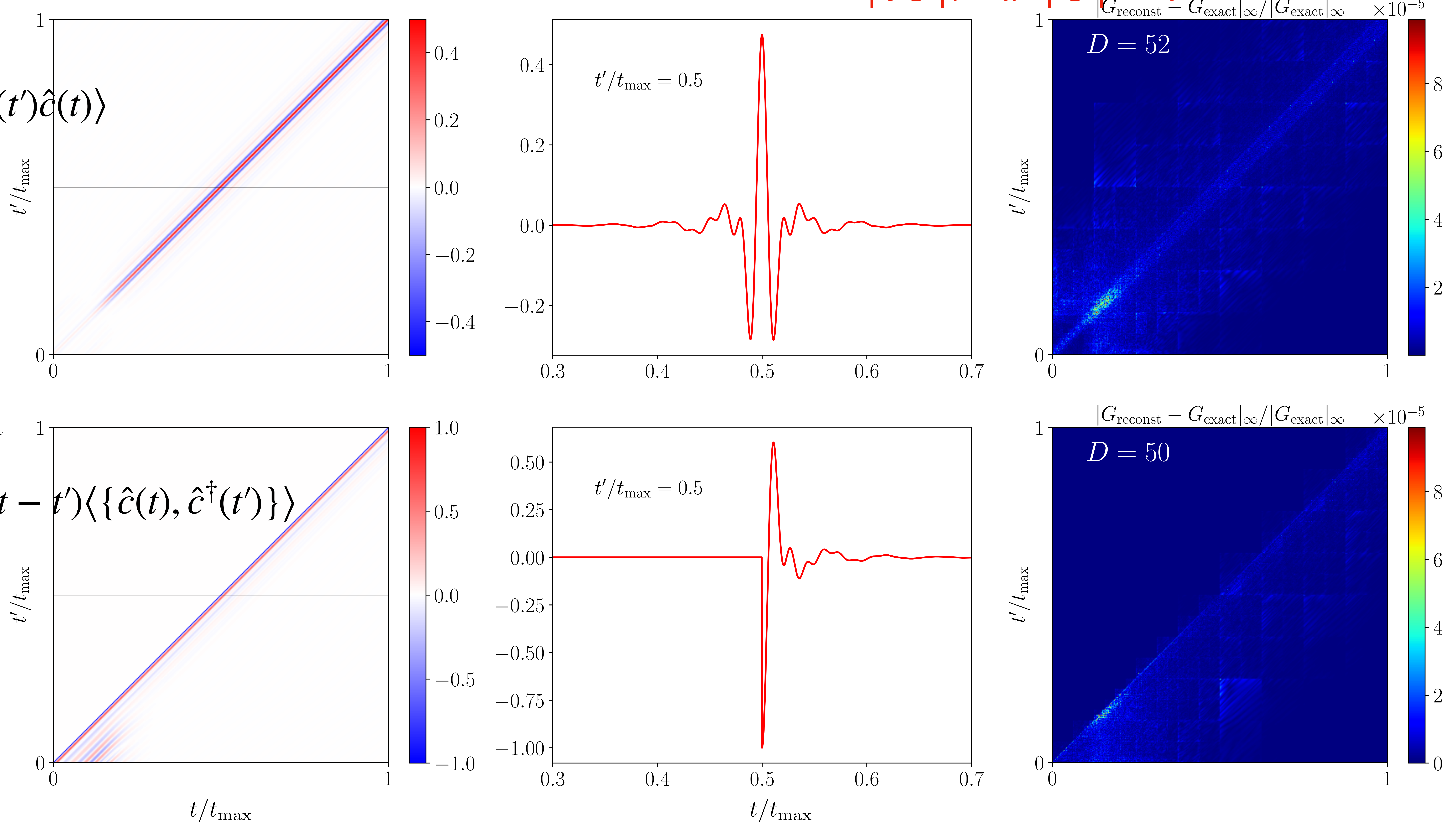
Low-T AF Mott phase excited by a short electric field pulse, Bethe lattice, $T = 0.05$

Compression ratio ~ 10^3

$|\delta G|/\max|G| \sim 10^{-3}$

$G^<(t,t') = i\langle \hat{c}^\dagger(t')\hat{c}(t)\rangle$

$G^R(t,t') = -i\theta(t-t')\langle\{\hat{c}(t),\hat{c}^\dagger(t')\}\rangle$



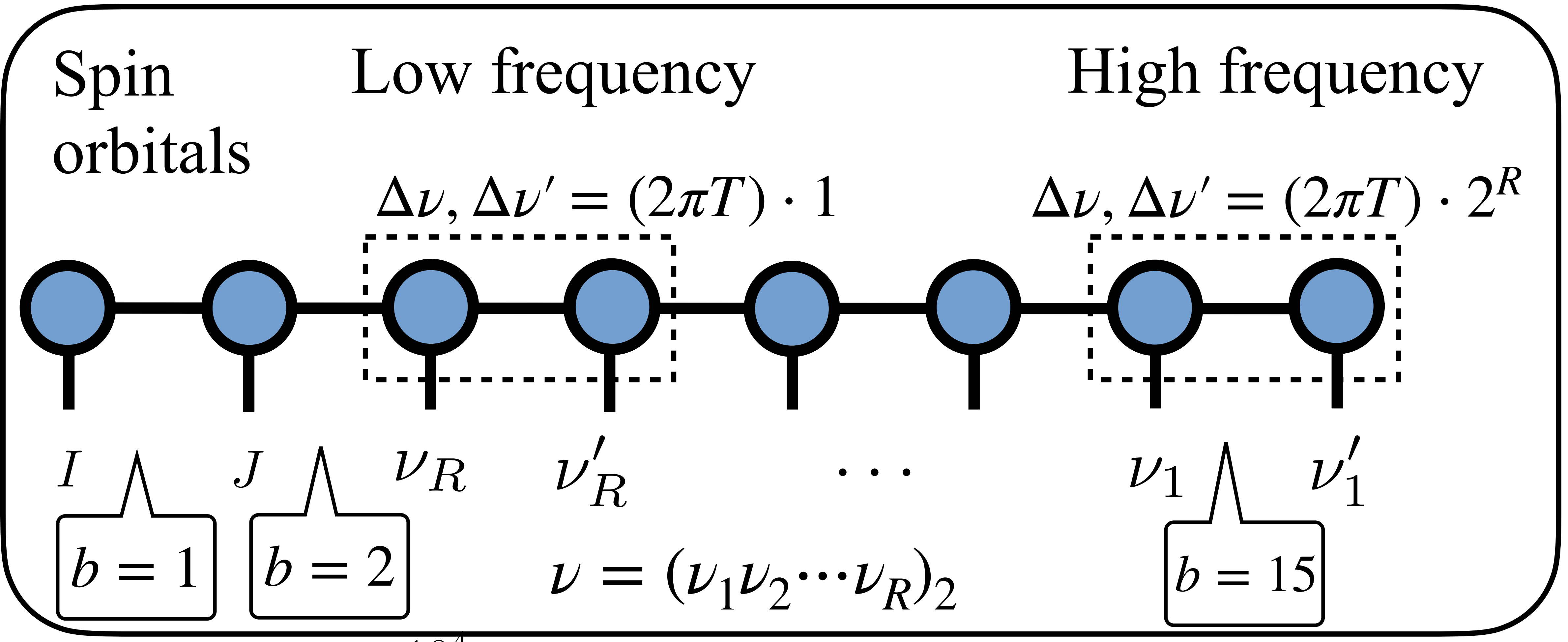
QTT is good at presenting diagonal structures!

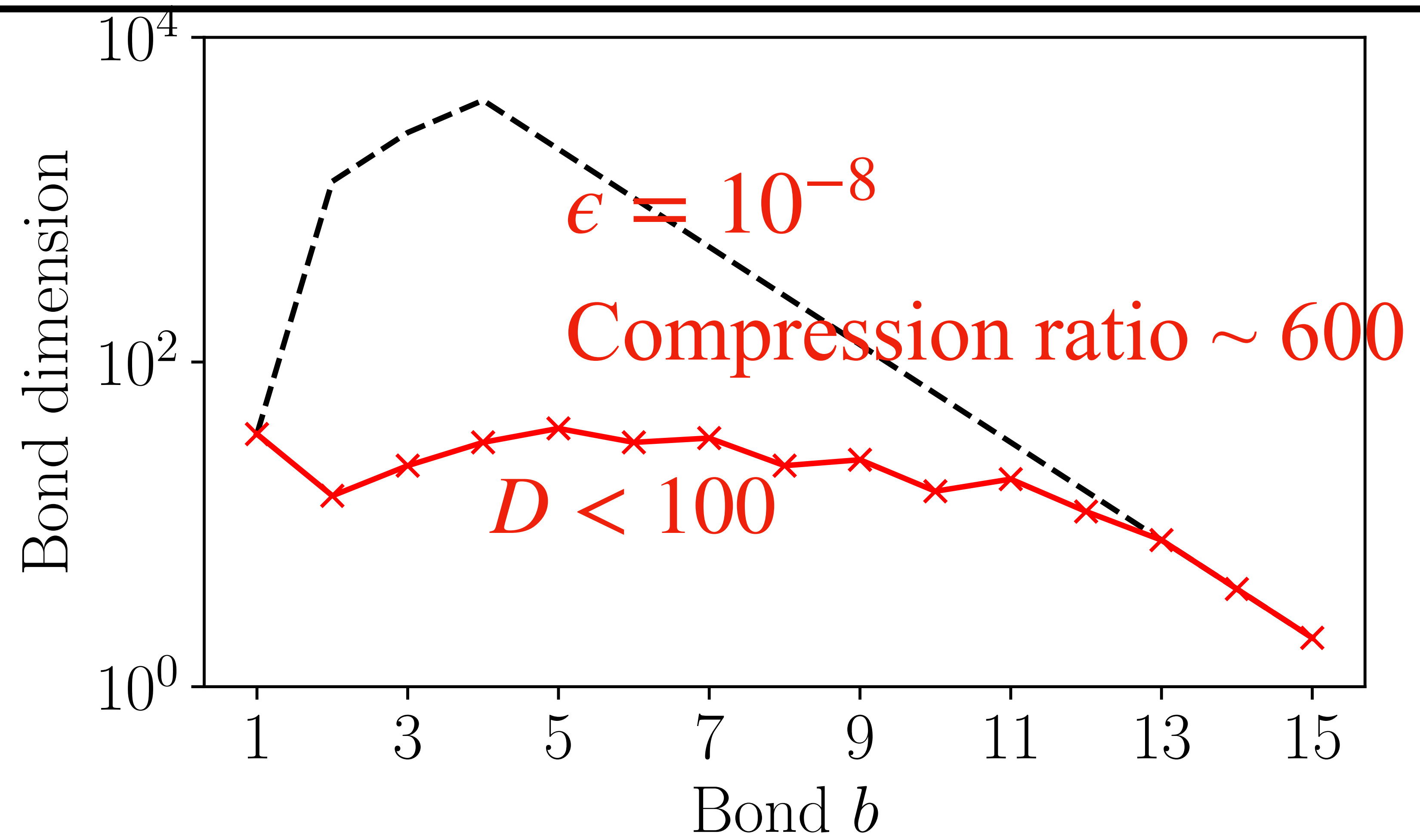
PRX **13**, 021015 (2023), arXiv:2303.11819

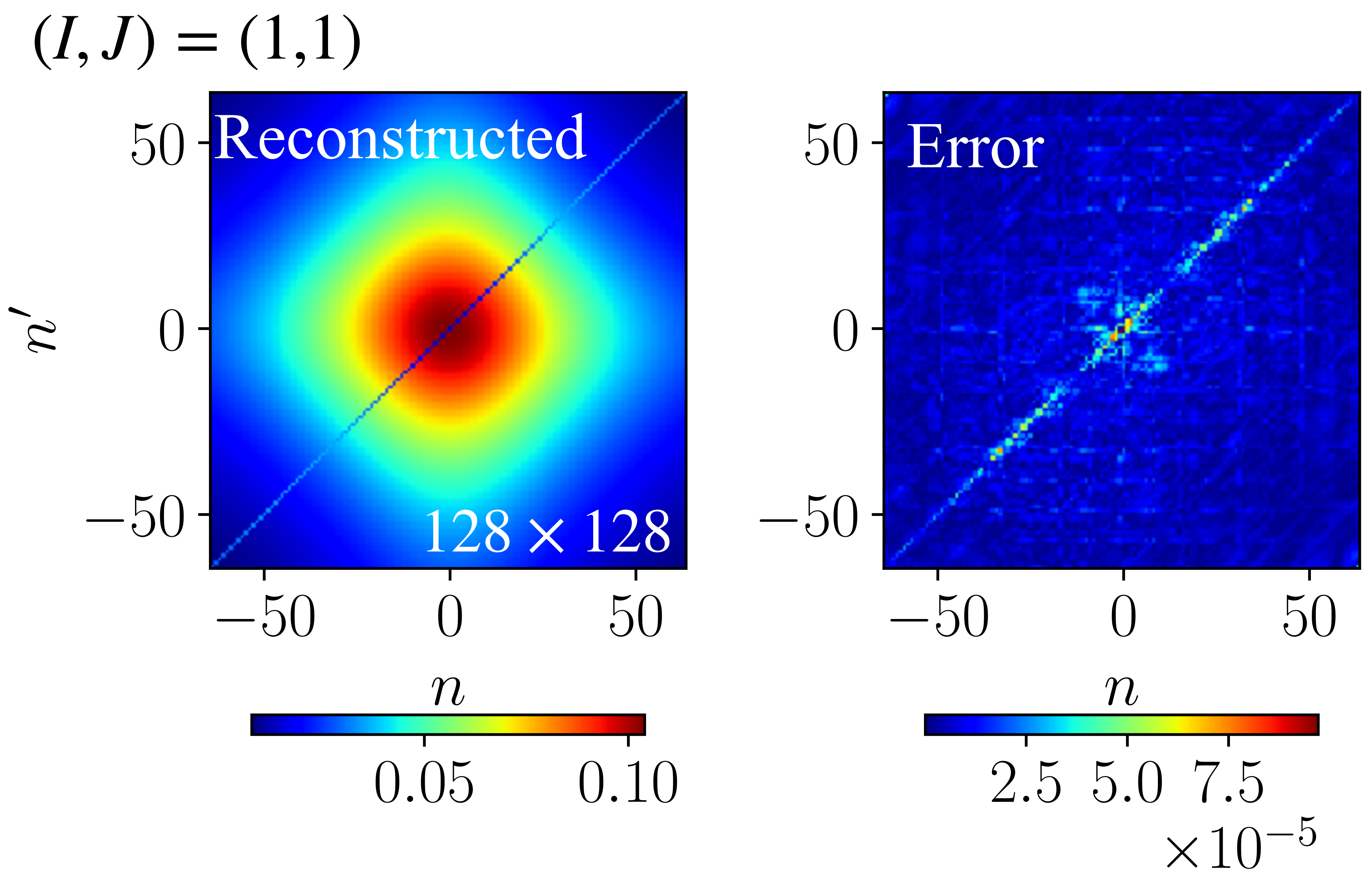
Multipolar susceptibility of an *f*-electron system: CeB_6

J. Otsuki, K. Yoshimi, **HS**, and H. O. Jeschke, arXiv:2209.10429v1

- Six correlated states (j=5/2)
- DFT+DMFT using the Hubbard-I approximation
- Static multipolar susceptibility computed by solving Bethe-Salpeter equation





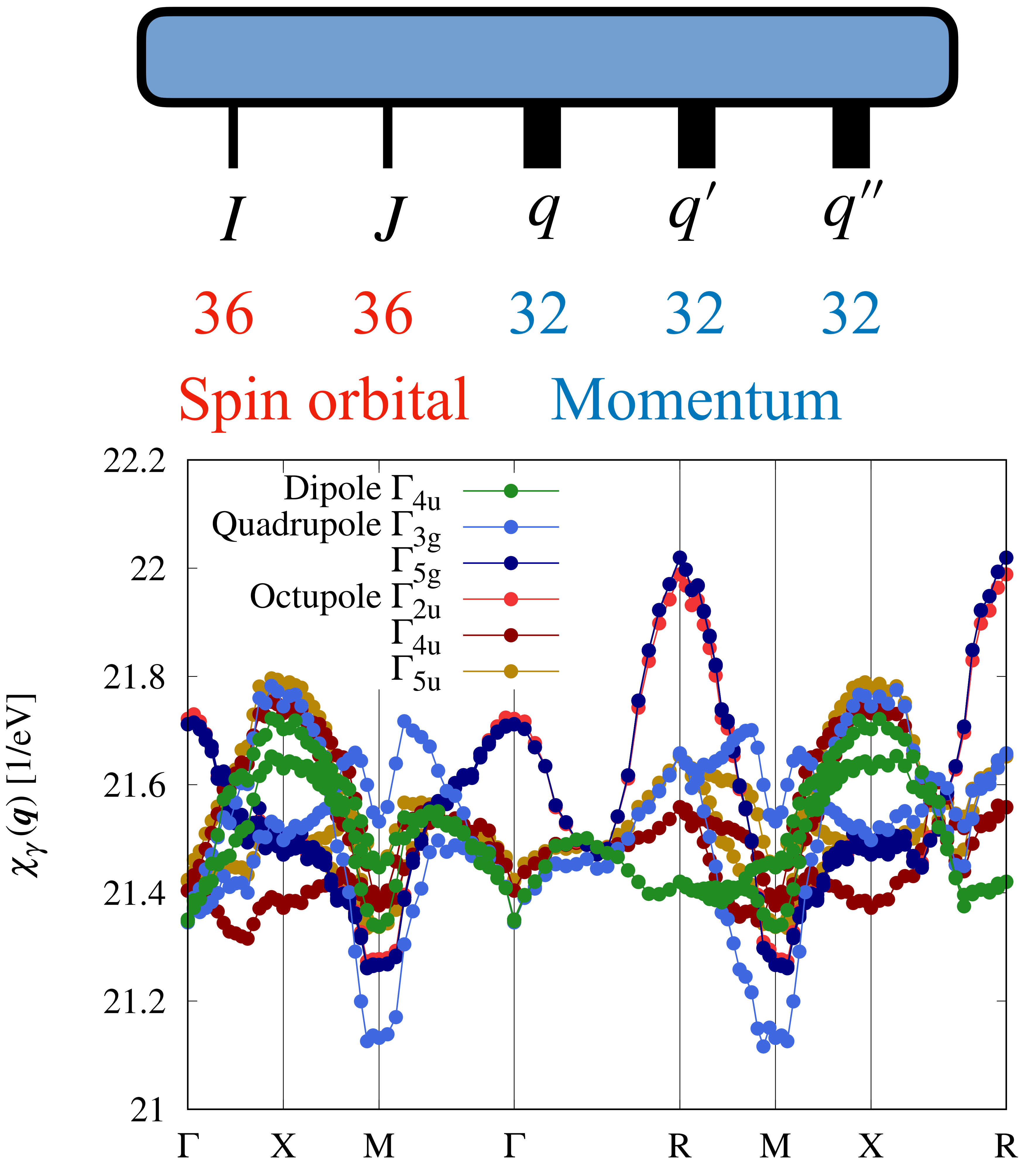


$\nu = (2n+1)\pi T,\ \nu' = (2n'+1)\pi T$

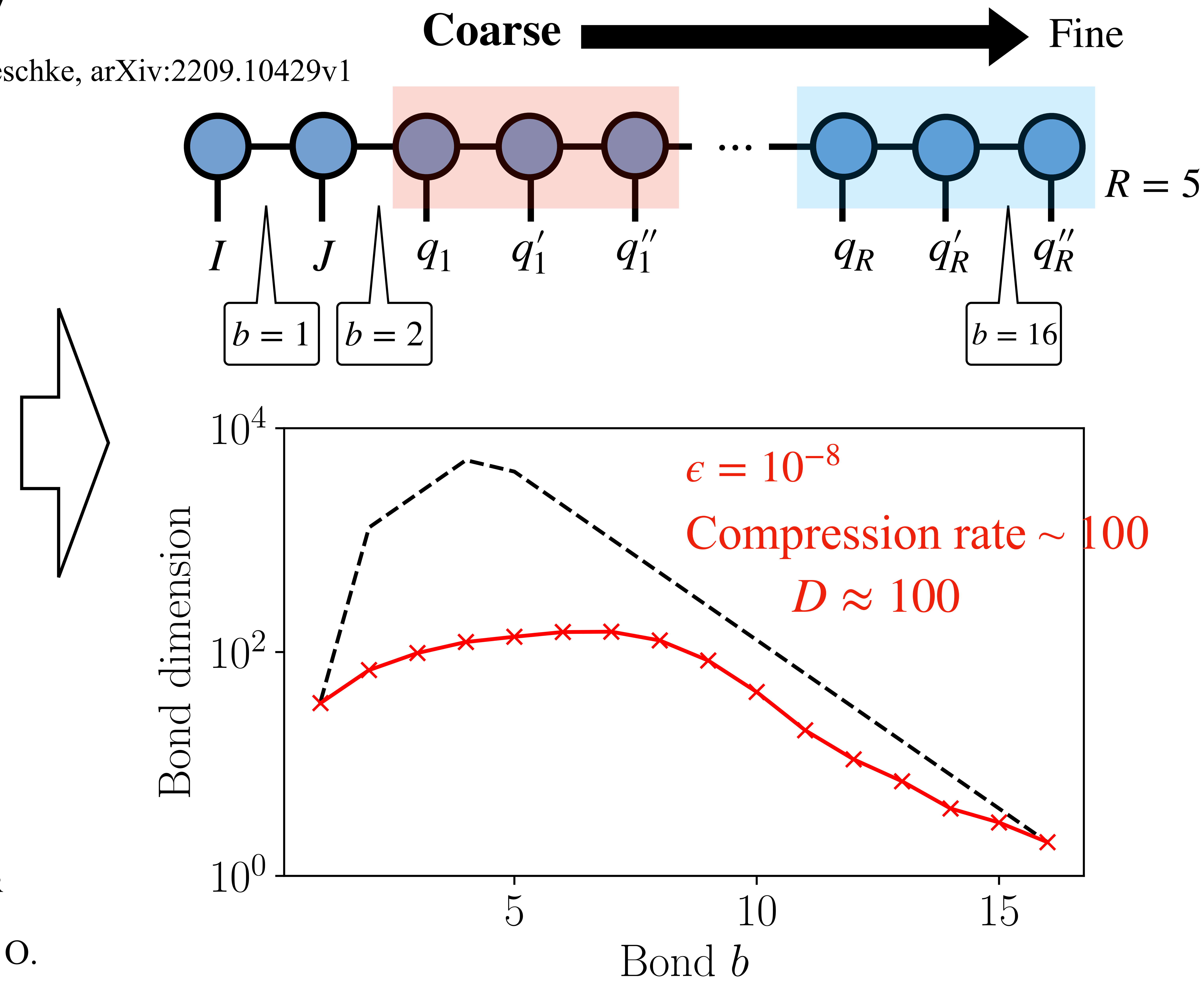
PRX **13**, 021015 (2023), arXiv:2303.11819

Multipolar susceptibility

J. Otsuki, K. Yoshimi, **HS**, and H. O. Jeschke, arXiv:2209.10429v1



J. Otsuki, K. Yoshimi, **HS**, and H. O. Jeschke, arXiv:2209.10429v1



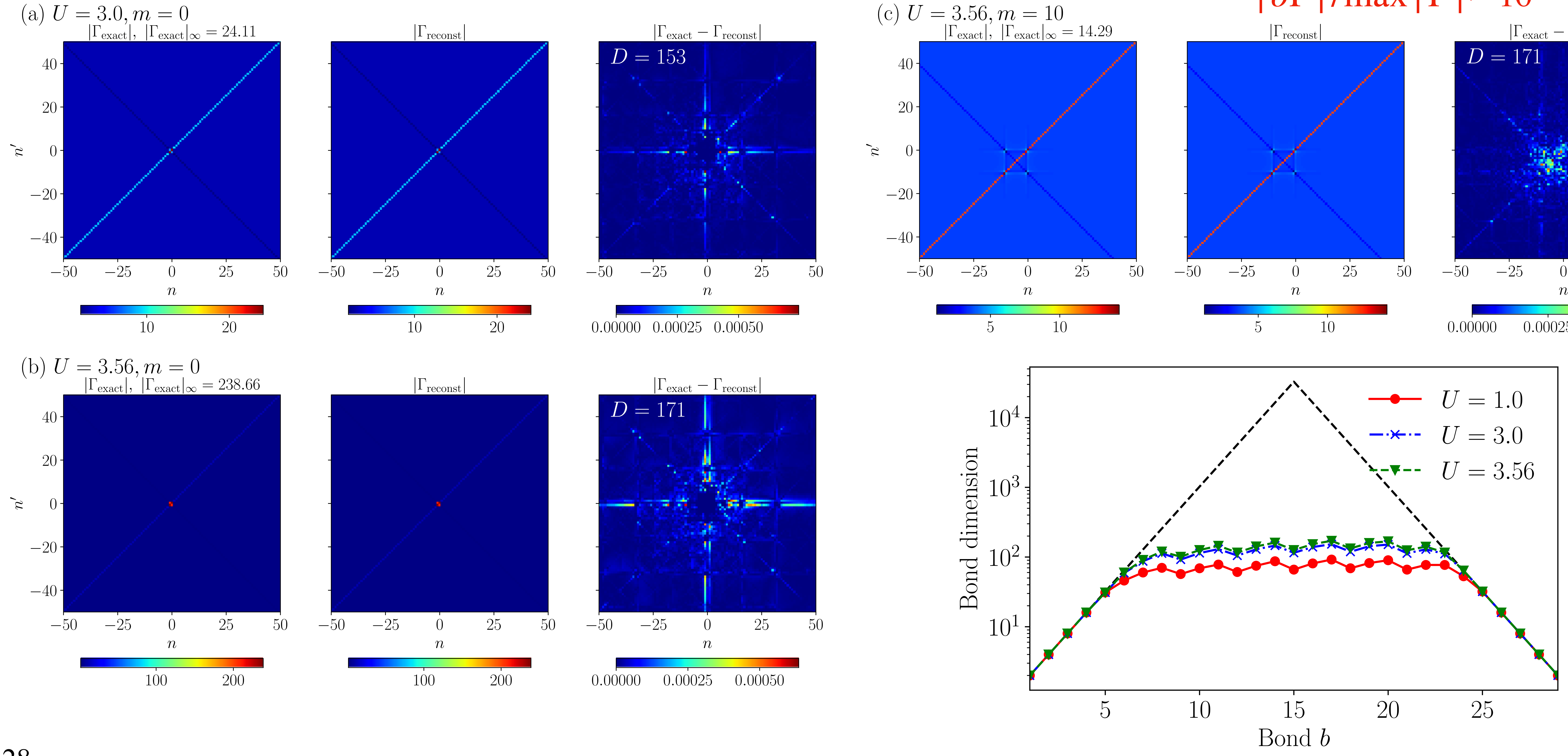
PRX **13**, 021015 (2023), arXiv:2303.11819

Three-frequency vertex function: Hubbard atom

Particle-hole & density channel, compressing three-frequency object

Compression rate ~ 10^3

$|\delta\Gamma|/\max|\Gamma| \sim 10^{-4}$



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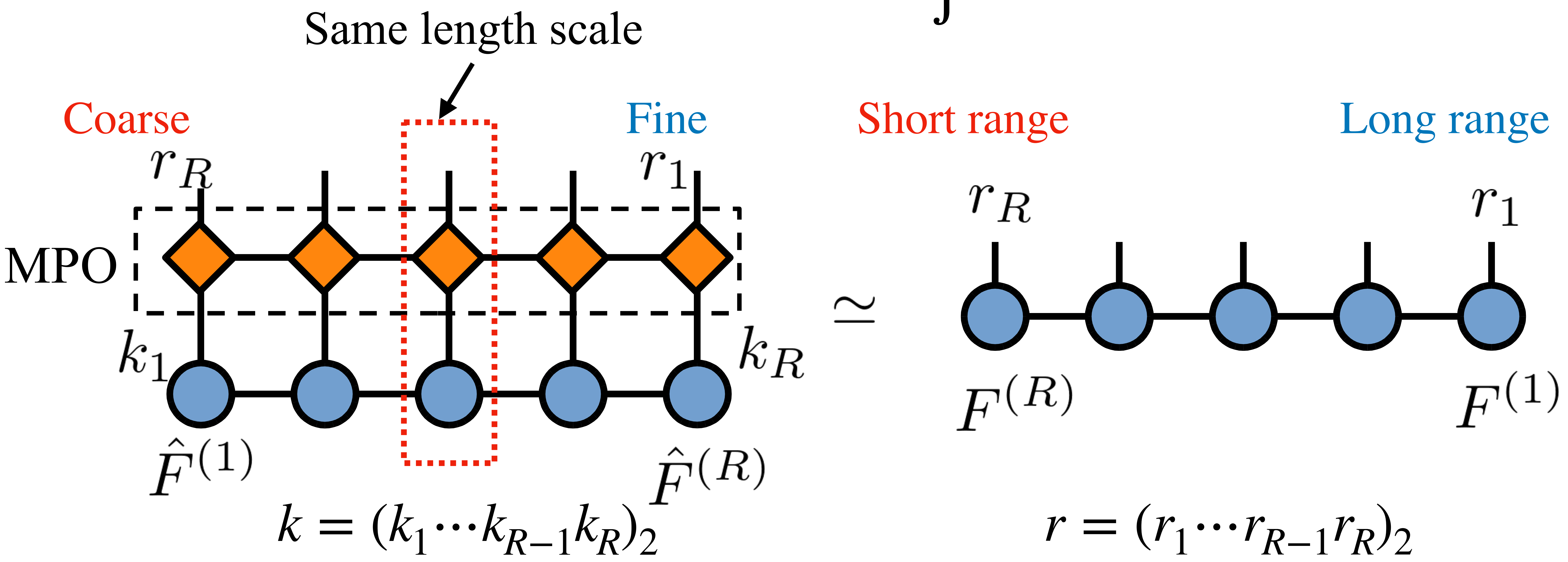
Computation

Quantum Fourier Transform

$$F(r) = \int \mathrm{d}k\ \hat{F}(k) e^{ikr}$$



Matrix product operator (MPO) can be constructed using quantum Fourier transform or discrete Fourier transform.

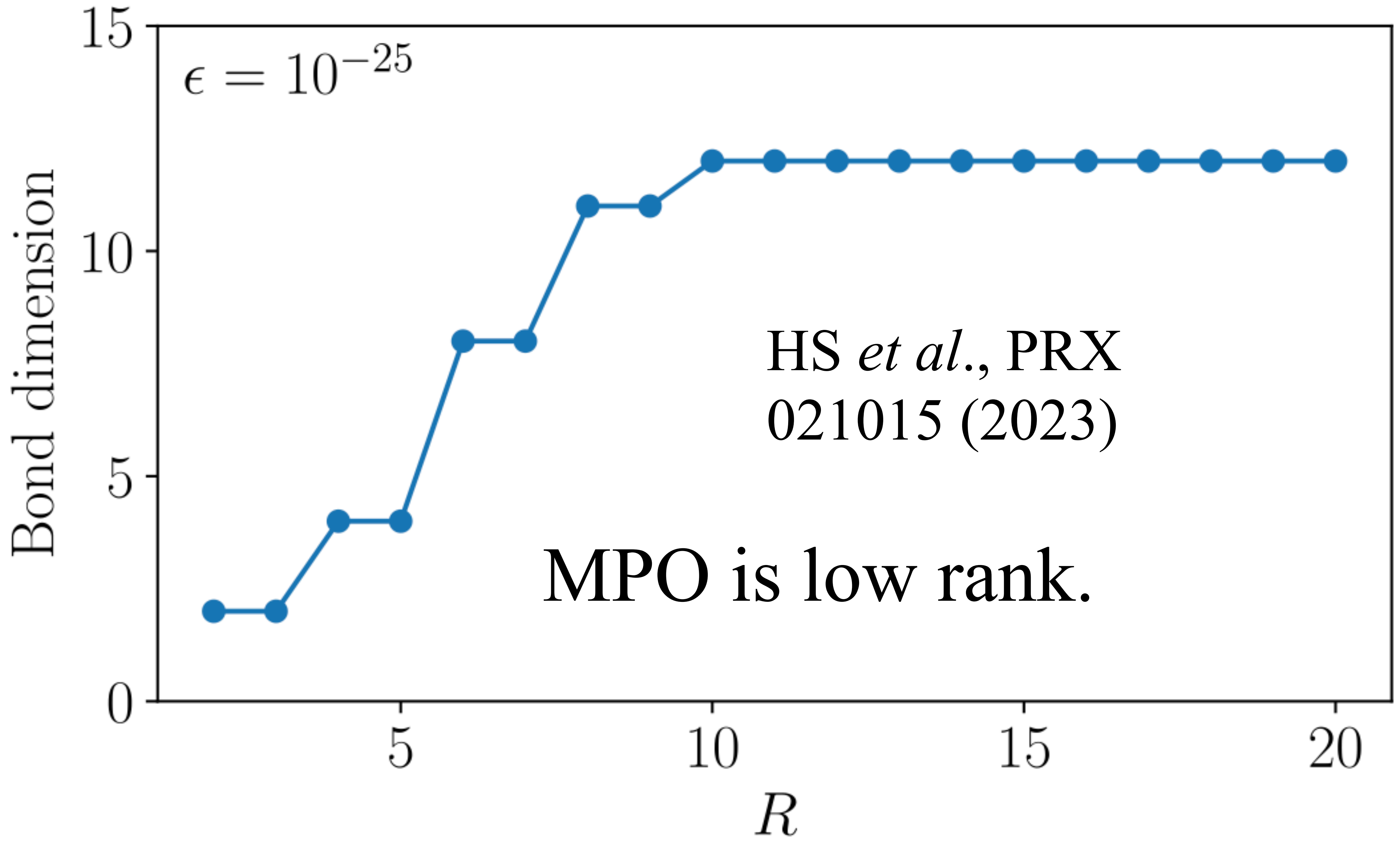
K. J. Woolfe *et al*., Quantum Inf. Comput. **17**, 1 (2017)

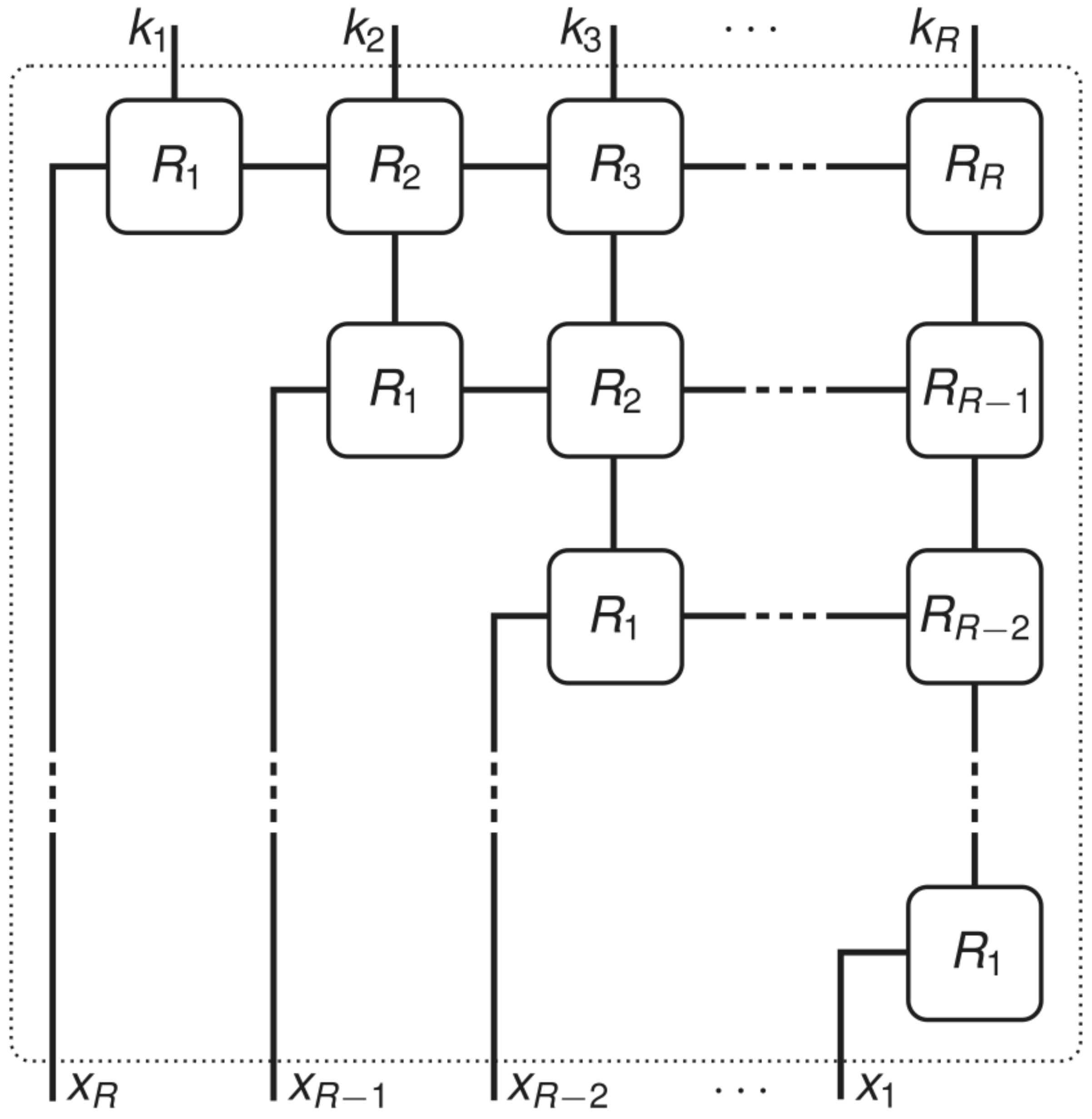
HS *et al*., PRX 021015 (2023)

J. Chen, E.M. Stoudenmire, S. R. White, arXiv:2210.08468v

Quantum Fourier Transform

$$F(r) = \int \mathrm{d}k \ \hat{F}(k) e^{\mathrm{i}kr}$$





Quantum Fourier transform can be simulated on a classical computer efficiently!

∵Fourier transform is almost independent on different length scales.

K. J. Woolfe *et al.*, Quantum Inf. Comput. **17**, 1 (2017) [only numerical]

HS *et al.*, PRX 021015 (2023) [only numerical]

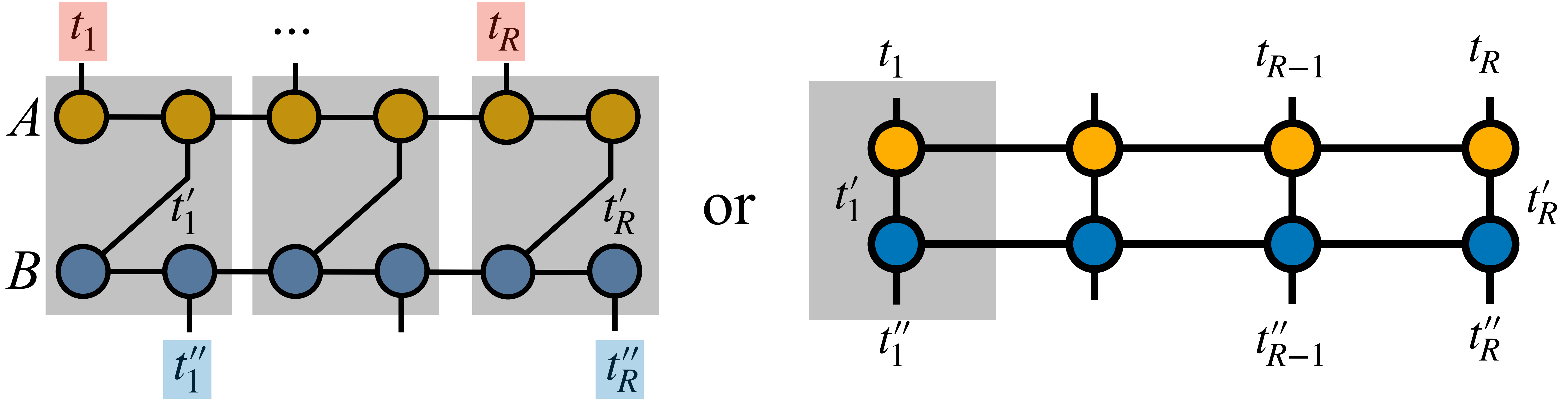
J. Chen, E.M. Stoudenmire, S. R. White, arXiv:2210.08468v1 [math proof]

PRX **13**, 021015 (2023), arXiv:2303.11819

Matrix multiplication/convolution

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

Tensor network contractions



If *A, B,* and *C* have a bond dimension of *D*, the computation time scales as $O(D^4)$.

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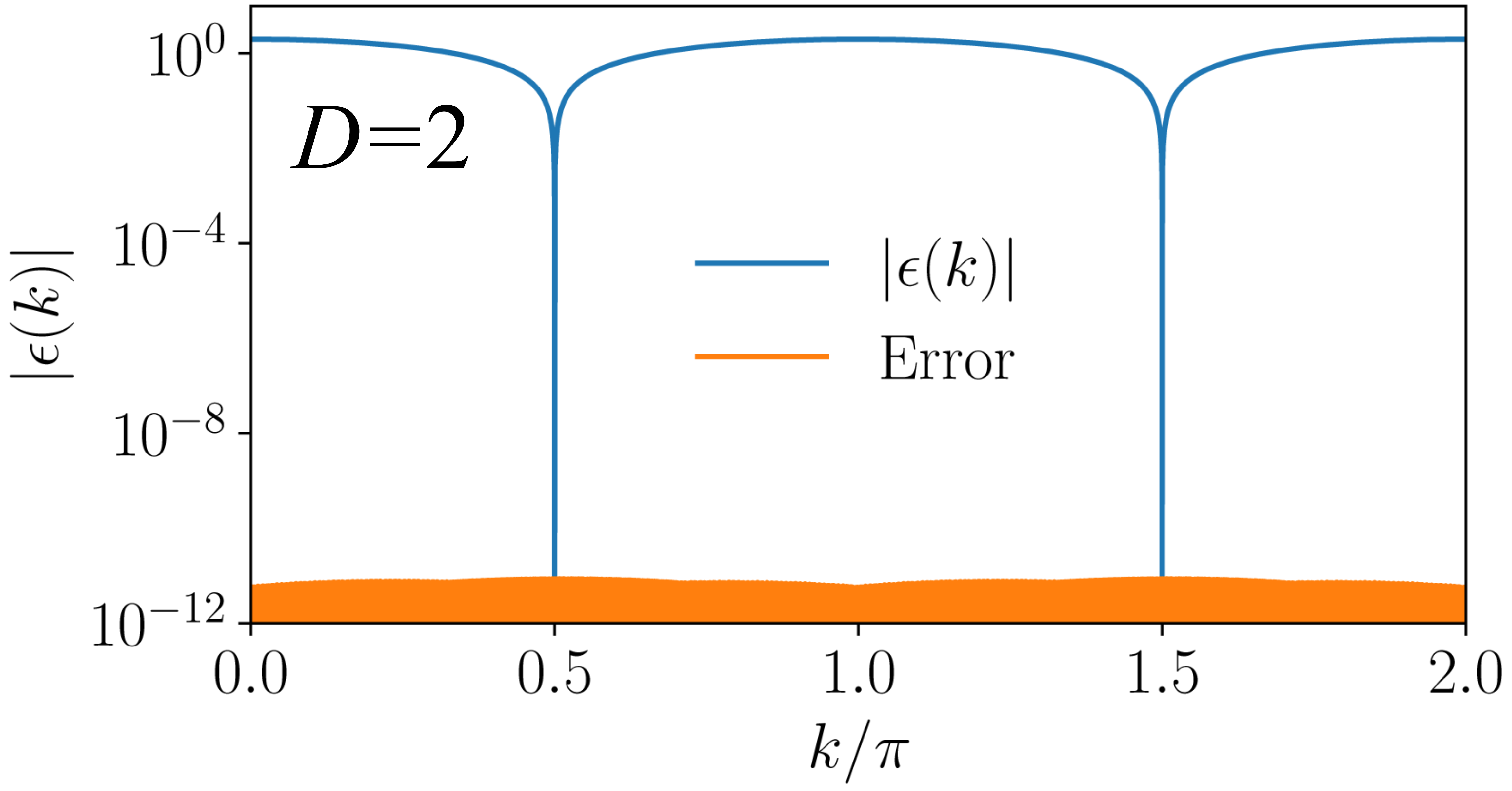
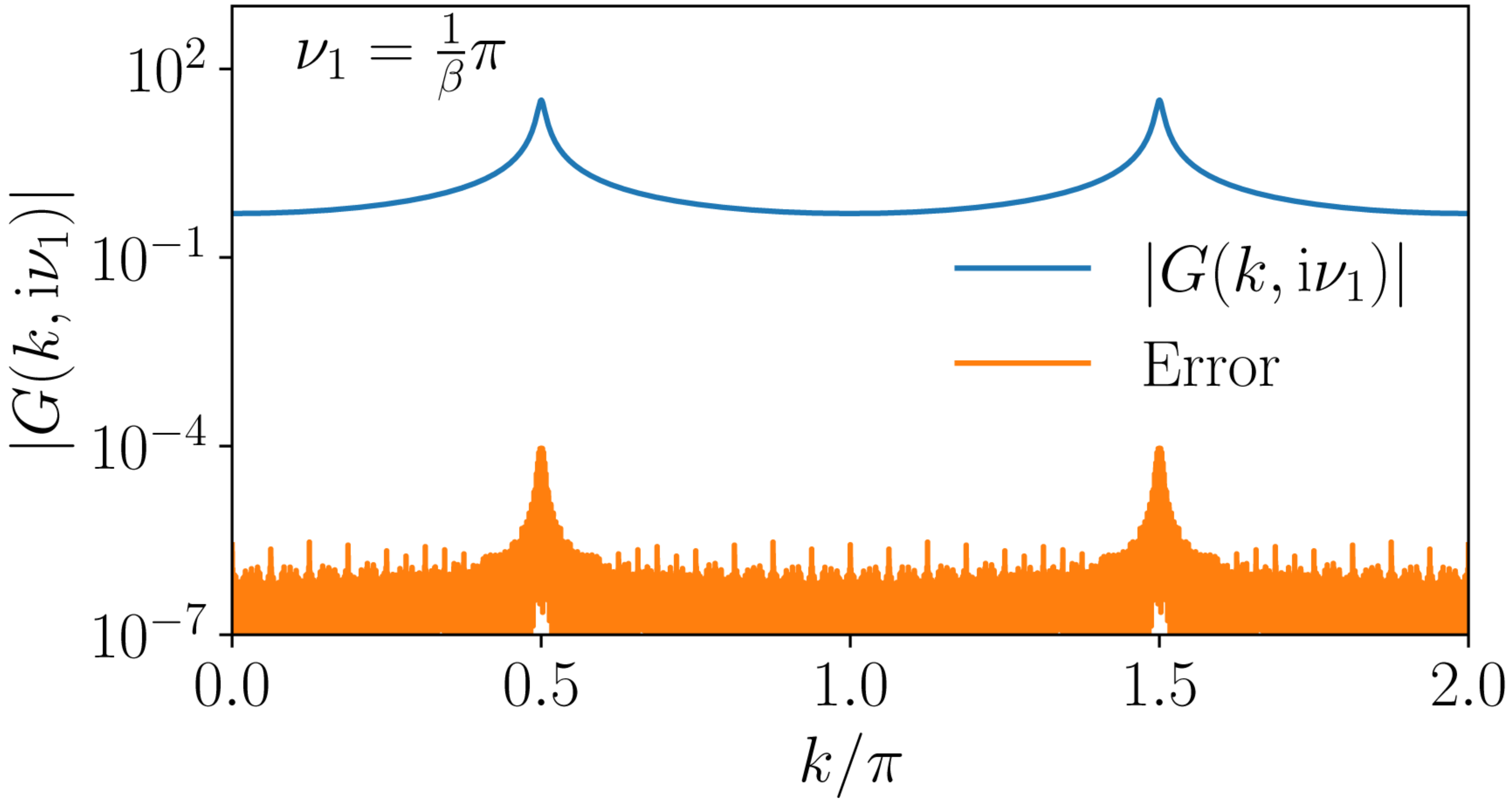
Dyson equation

1D tight-binding model $R = 20$ $(2^R \approx 10^6)$, $\beta = 100$

$\epsilon(r)$ → QFT → $\epsilon(k)$ → $(\mathrm{i}\nu - \epsilon(k))G(k, \mathrm{i}\nu) = 1$ (Krylov method) → $G(k, \mathrm{i}\nu)$





Exponential speed up

In practice, quantics TCI is more efficient (Part II).

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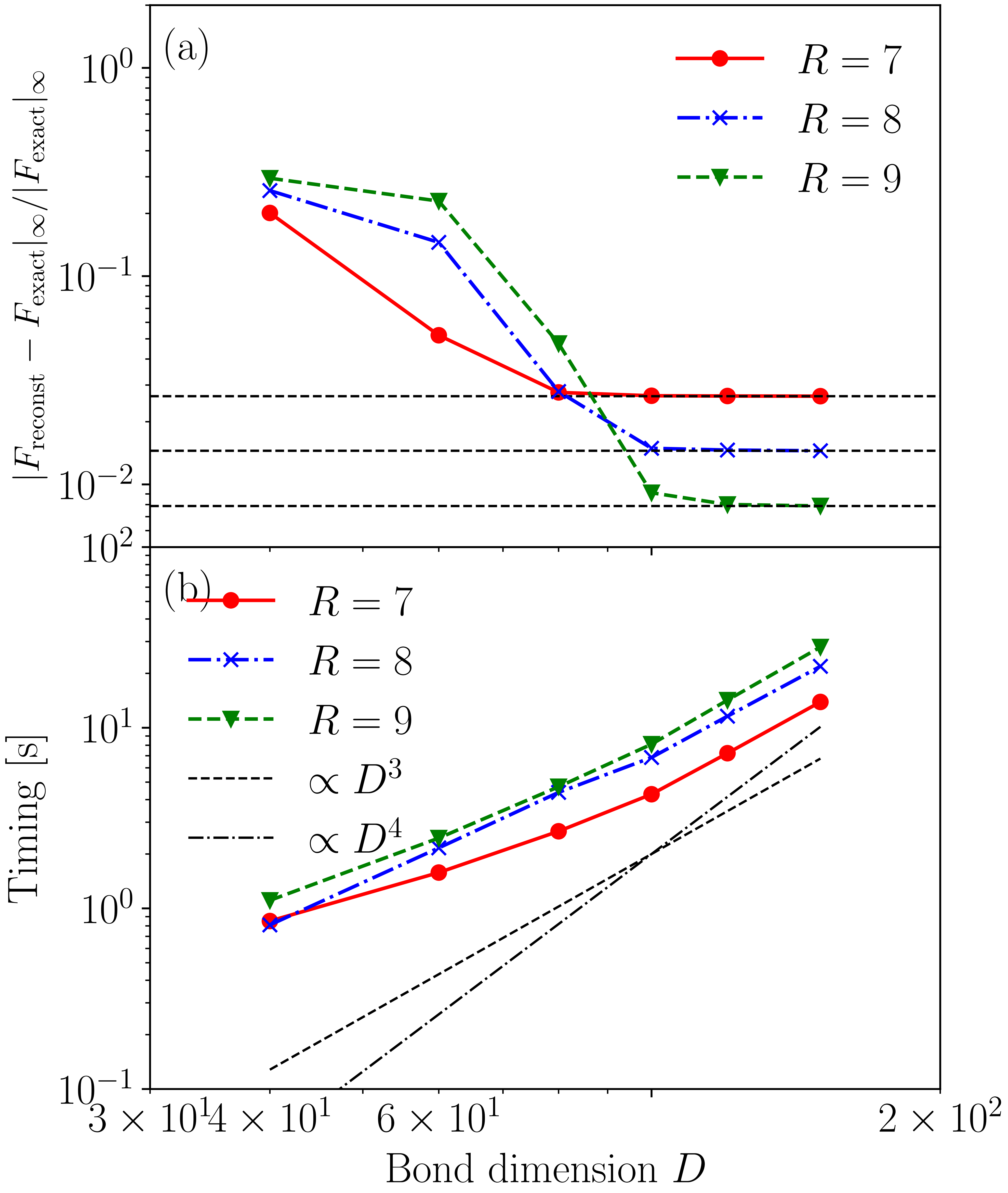
Bethe-Salpeter equation

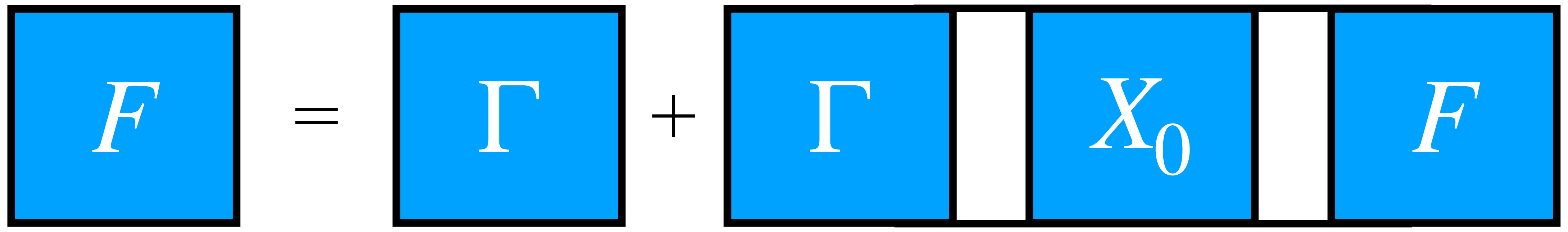
Particle-hole & density channel



Hubbard atom, U=3, β=1

One-shot evaluation of BSE in three-frequency space

$$F_{\text{reconst}} = \Gamma + (\beta^{-2}(\Gamma(X^0 F)))$$



$$F_{d/m}(\mathrm{i}\nu, \mathrm{i}\nu'; \mathrm{i}\omega) = \Gamma_{d/m}(\mathrm{i}\nu, \mathrm{i}\nu'; \mathrm{i}\omega)$$
$$+ \frac{1}{\beta^2} \sum_{\nu'', \nu'''} \Gamma_{d/m}(\mathrm{i}\nu, \mathrm{i}\nu''; \mathrm{i}\omega) X^0(\mathrm{i}\nu'', \mathrm{i}\nu'''; \mathrm{i}\omega)$$
$$\times\ F_{d/m}(\mathrm{i}\nu''', \mathrm{i}\nu'; \mathrm{i}\omega),$$

Exponential speed up

PRX **13**, 021015 (2023), arXiv:2303.11819

Outline

- Introduction
- Part I Quantics tensor train

  HS *et al*., PRX **13**, 021015 (2023)
- Part II Quantics tensor cross interpolation

  M. K. Ritter, Y. N. Fernández, M. Wallerberger, J. von Delft, **HS**, X. Waintal, arXiv:2303.11819
- Outlook & summary

Different routes to quantics

1. Analytic form: exponential
2. SVD of numerical data
3. Computation on the fly: Dyson, Bethe-Salpeter equations.
4. Quantics Tensor Cross Interpolation

M. K. Ritter, Y. N. Fernández, M. Wallerberger, J. von Delft, HS, X. Waintal, arXiv:2303.11819

Learning a compressed representation from a few function evaluations
Matrix/tensor cross interpolation

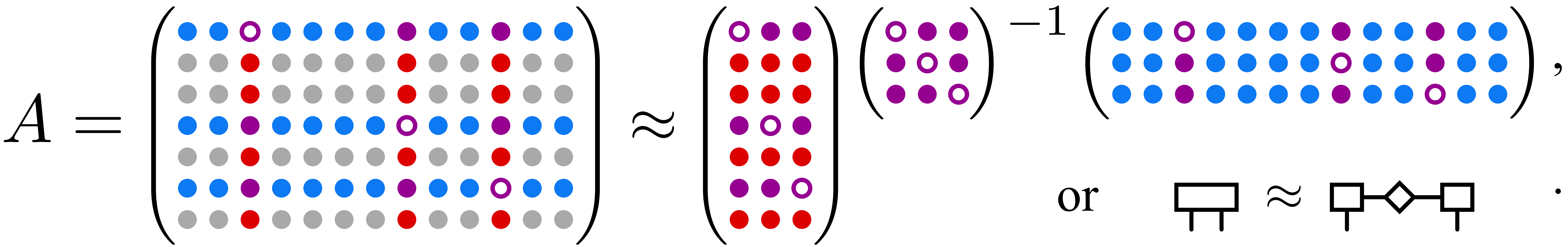
PRX **13**, 021015 (2023), arXiv:2303.11819

Matrix Cross Interpolation (MCI)

Review: N. Kishore Kumar and J. Schneider, Linear Multilinear Alg. **65**, 2212 (2017)

Problem Low-rank approximation of a matrix A by SVD requires knowing all the matrix elements….

MCI $A \approx CP^{-1}R = \tilde{A}$ Selected rows Crosses Selected columns



- No need to read all elements of a low-rank matrix!
- Equality is exact on the selected columns and rows.
- Many algorithms to choose good pivots:
  e.g., Maxvol (maximize |P|)

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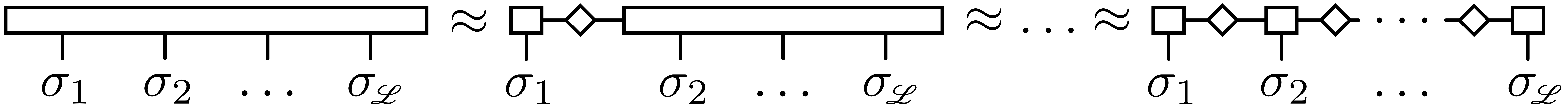
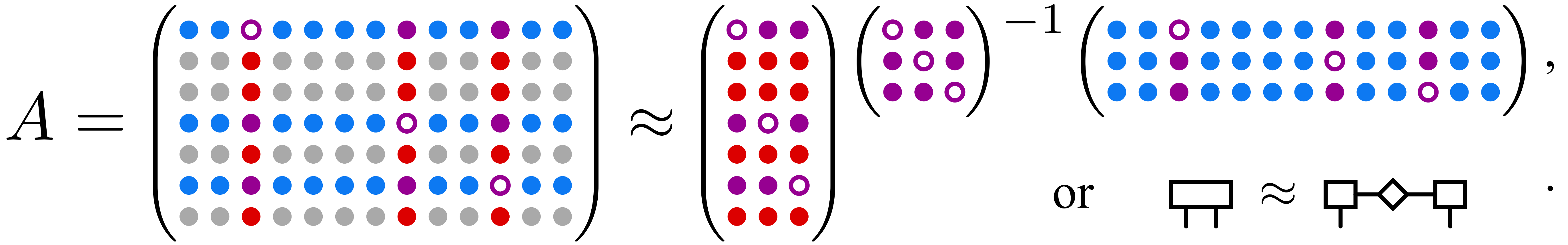
Tensor cross interpolation (TCI)

I. V. Oseledets, SIAM Journal on Scientific Computing **33**, 2295 (2011)

S. Dolgov and D. Savostyanov, Computer Physics Communications **246**, 106869 (2020)





\# of function evaluations $\propto$ # of elements in the tensors $\propto O(D^2)$

- Function evaluation on the fly
- No need to store all tensor elements

TCI is general and is ready to work with quantics!

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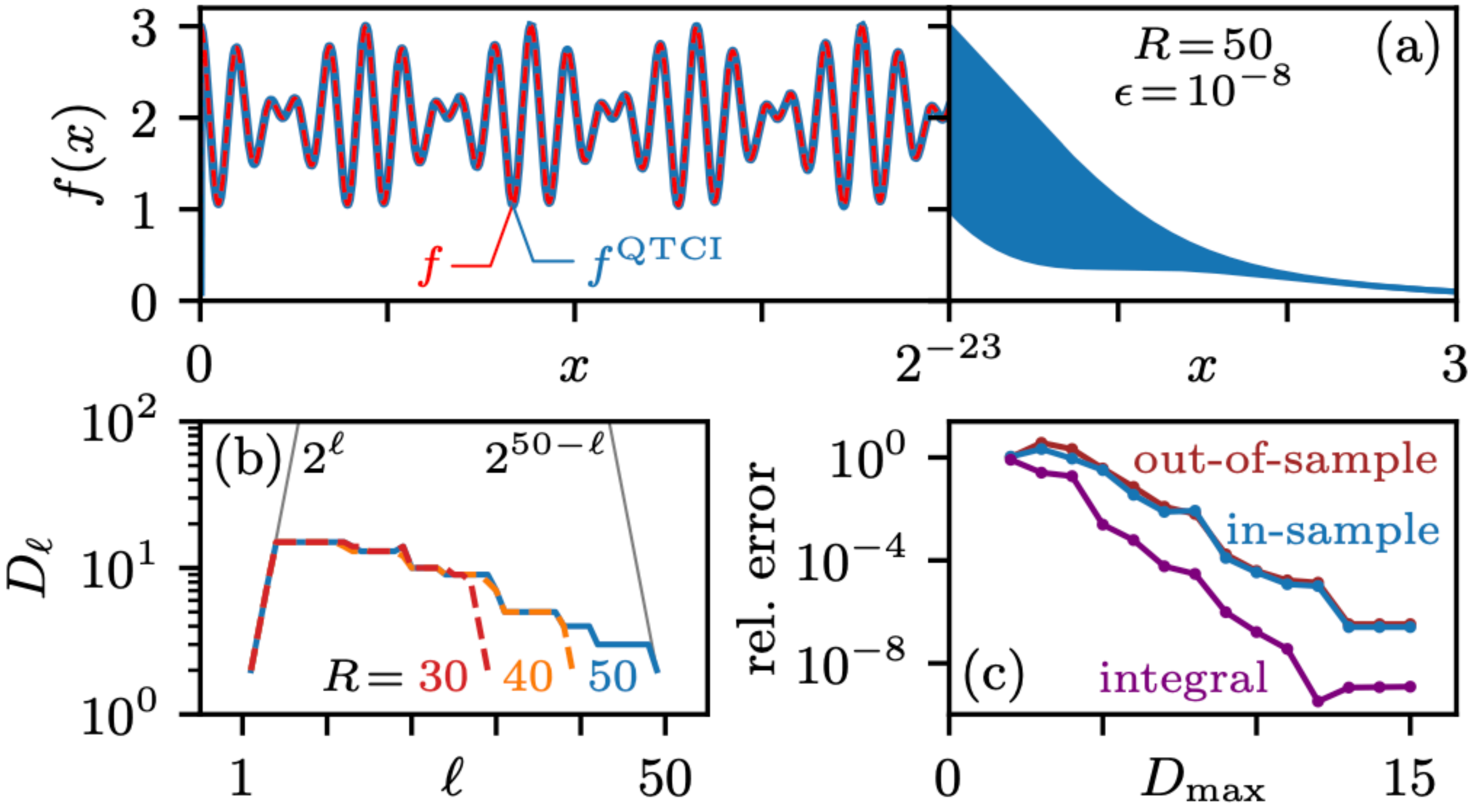
1D integration

M. K. Ritter, Y. N. Fernández, M. Wallerberger, J. von Delft, HS, X. Waintal, arXiv:2303.11819

$$f(x) = \cos\left(\frac{x}{B}\right)\cos\left(\frac{x}{4\sqrt{5}B}\right)e^{-x^2} + 2e^{-x} \text{ with } B = 2^{-30} \approx 10^{-9}.$$

Fast oscillations Slow decay

$$\int_0^{\ln(20)} dx f(x) = \frac{19}{10} + O(e^{-1/(4B^2)})$$



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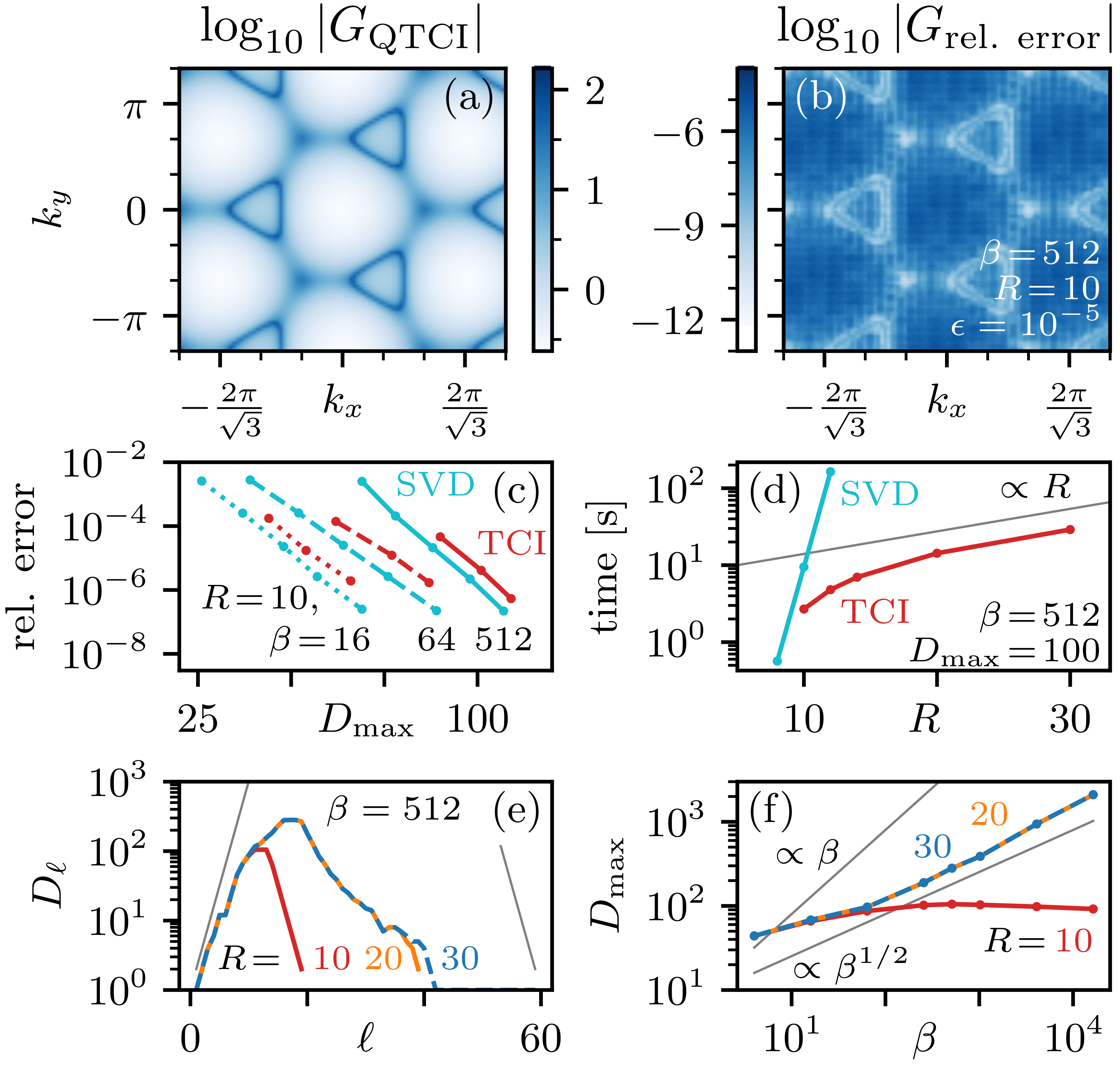
Momentum dependence of single-particle Green's function

M. K. Ritter, Y. N. Fernández, M. Wallerberger, J. von Delft, HS, X. Waintal, arXiv:2303.11819

μ is shifted from half filling.



Haldane model

$$H(\vec{k}) = \sum_{i=1}^{3}\left[\sigma^1\cos(\vec{k}\cdot\vec{a}_i)+\sigma^2\sin(\vec{k}\cdot\vec{a}_i)\right]+\sigma^3\left[m-2t_2\sum_{i=1}^{3}\sin(\vec{k}\cdot\vec{b}_i)\right],$$

- Exponential convergence
- QTCI is quasi-optimal (for ranks).
- QTCI is exponentially faster than SVD.
- Bond dimension grows only as $O(\beta^{1/2})$ for 2D.

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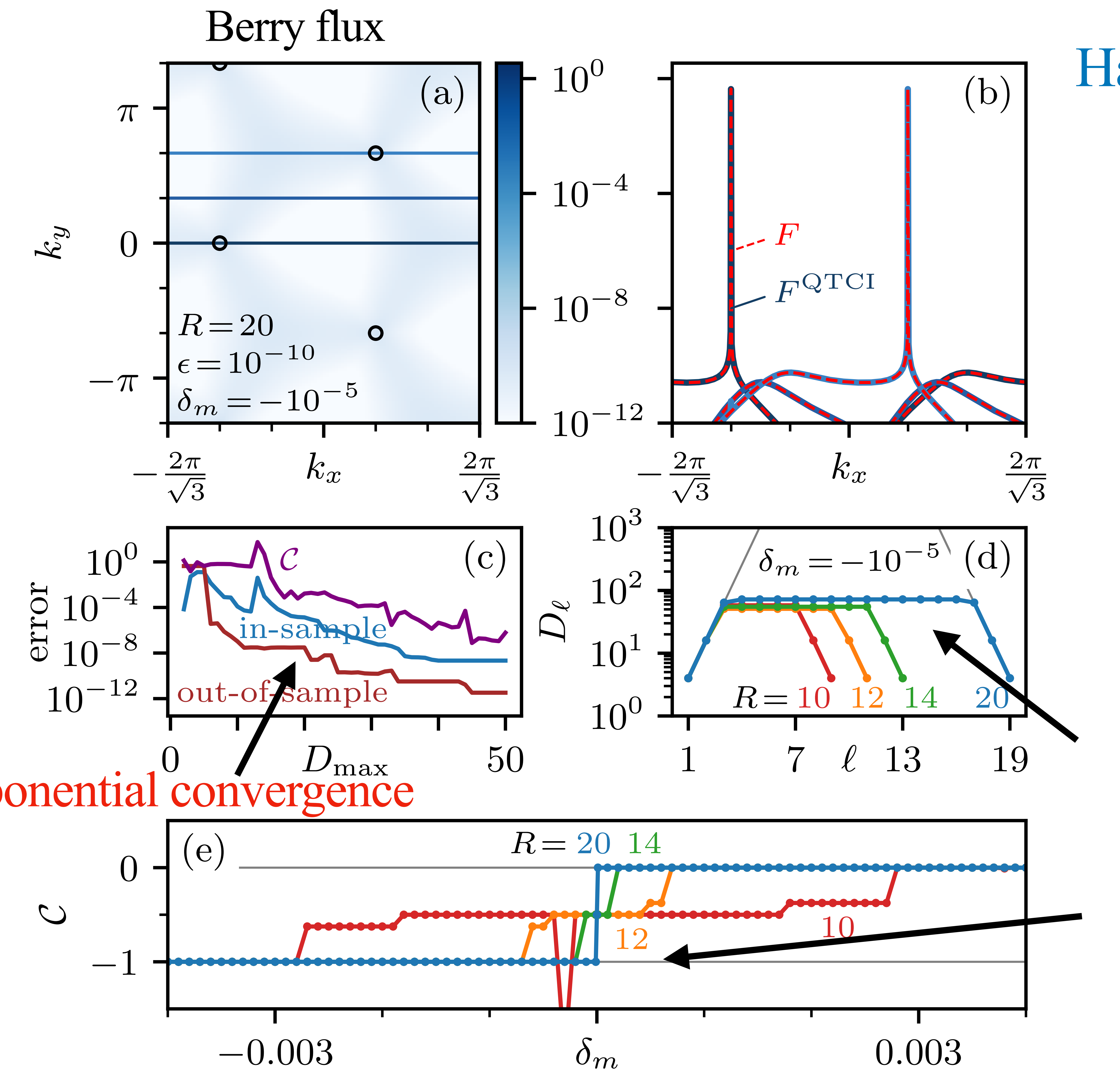
Chern number

M. K. Ritter, Y. N. Fernández, M. Wallerberger, J. von Delft, HS, X. Waintal, arXiv:2303.11819



Exponential convergence

Haldane model

$$H(\vec{k}) = \sum_{i=1}^{3}\left[\sigma^1\cos(\vec{k}\cdot\vec{a}_i)+\sigma^2\sin(\vec{k}\cdot\vec{a}_i)\right]+\sigma^3\left[m-2t_2\sum_{i=1}^{3}\sin(\vec{k}\cdot\vec{b}_i)\right],$$

$\delta_m = m - m_c$: deviation from a topological transition

$$\mathcal{C} \approx \frac{1}{2\pi i}\sum_{\vec{k}\in\mathrm{BZ}} F(\vec{k})$$

summation of Berry flux over plaquettes

$$F(\vec{k}) \approx -i\arg\left(\langle\psi_{\vec{k}_1}|\psi_{\vec{k}_2}\rangle\langle\psi_{\vec{k}_2}|\psi_{\vec{k}_3}\rangle\langle\psi_{\vec{k}_3}|\psi_{\vec{k}_4}\rangle\langle\psi_{\vec{k}_4}|\psi_{\vec{k}_1}\rangle\right)$$

Separation in length scale

Exponentially precisely determination with increasing the number of bits R

PRX **13**, 021015 (2023), arXiv:2303.11819

Outlook

QTT + TCI could be a general framework to attack many problems.

Ab initio calculations

Quantum impurity solvers without sign problem

Diagrammatic calculations at the two-particle level

More general tensor networks

Tree tensor network, PEPS…

Applied math aspects

Comparison with adaptive grids, more robust TCI algorithms

Open-source software

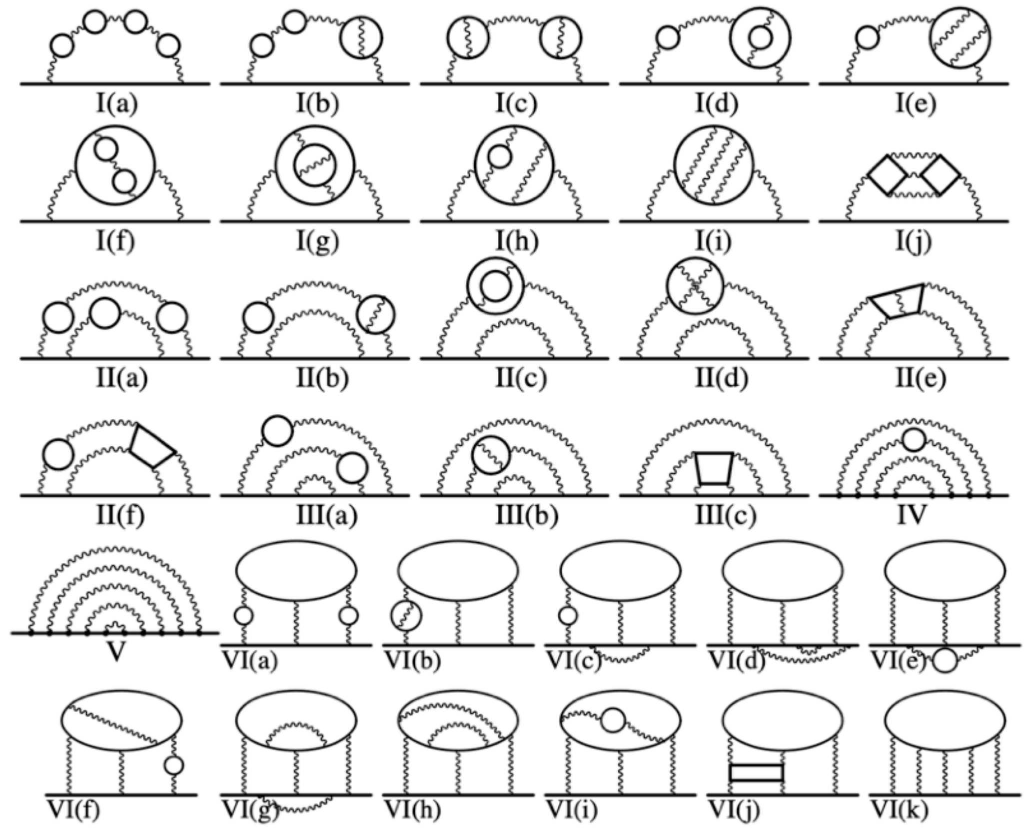
Will be published soon

Beyond condensed matter physics?

Cosmic strings

Plank scale width vs universe-scale length

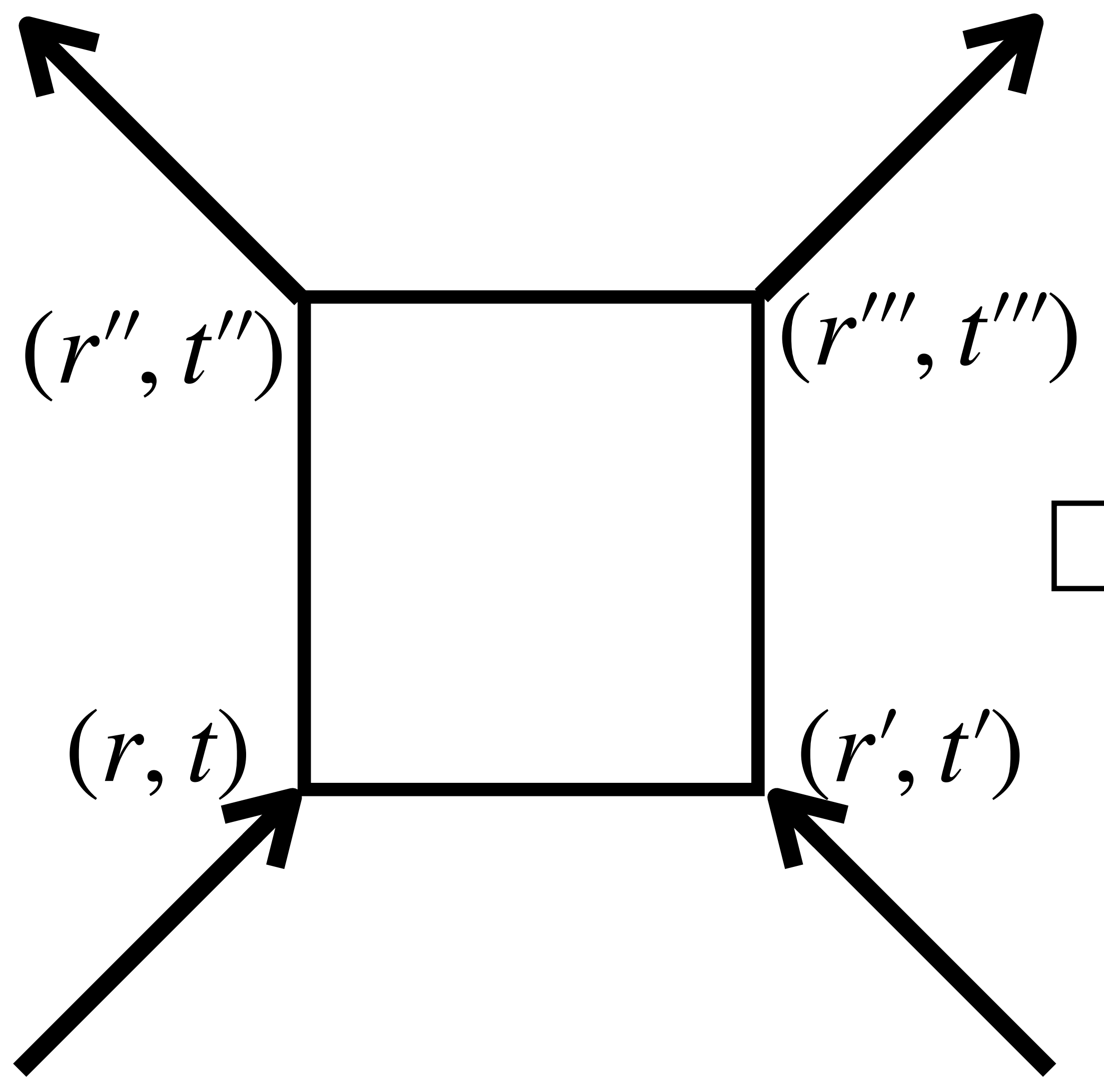
Perturbation theory in QED



T. Aoyama, T. Kinoshita, M. Nio, Atoms **7**, 28 (2019)

PRX **13**, 021015 (2023), arXiv:2303.11819

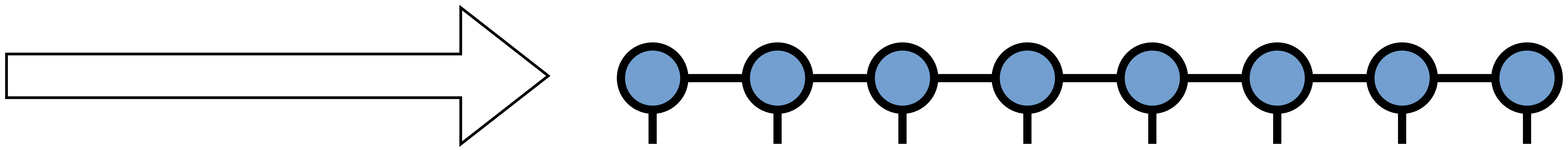
Summary



① Quantics tensor train

HS *et al.*, PRX **13**, 021015 (2023)

Representing features across widely (exponentially) different length scales



Computation in compressed form: Fourier transform, convolution…

② Quantics tensor cross interpolation

M. K. Ritter, Y. N. Fernández, M. Wallerberger, J. von Delft, **HS**, X. Waintal, arXiv:2303.11819

Learning such a representation from a function
Applications: BZ/time integration…

PRX **13**, 021015 (2023), arXiv:2303.11819