# Quantics tensor trains and many-body physics

Hiroshi SHINAOKA

Saitama University

HS, M. Wallerberger, Y. Murakami, K. Nogaki, R. Sakurai, P. Werner, A. Kauch, arXiv:2210.12984v2 (to appear in PRX)
M. K. Ritter, Y. N. Fernández, M. Wallerberger, J. von Delft, HS, X. Waintal, arXiv:2303.11819

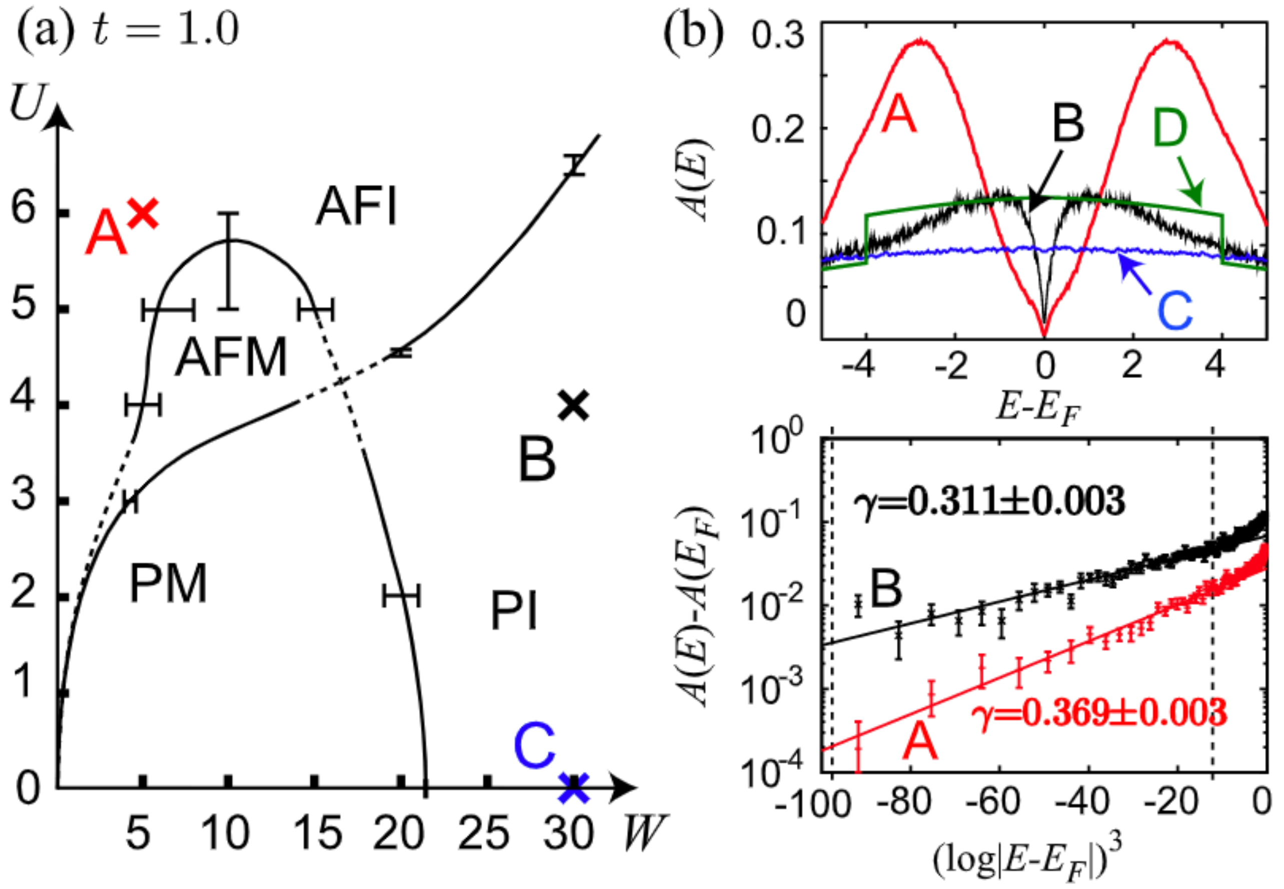
1. Inspired by quantum Fourier transform
2. Important for quantum-classical hybrid computation of solids



科研費 KAKENHI
PRESTO SAKIGAKE

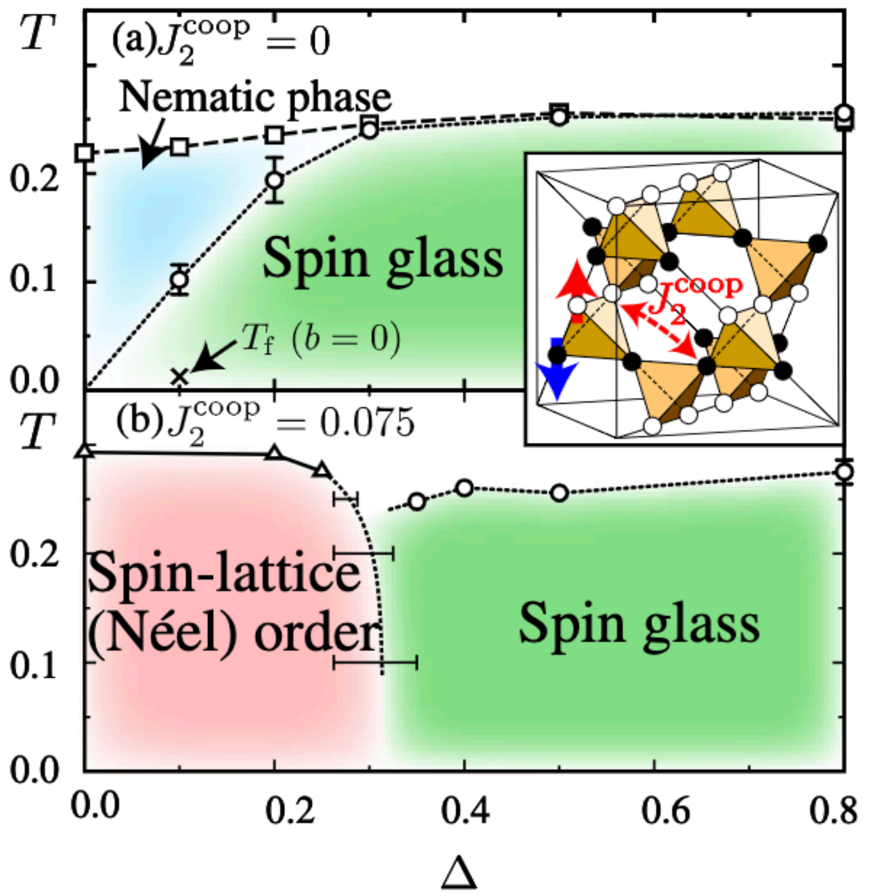
# Introduction　元々は複雑な強相関物理の理解に興味がある

## 強相関系におけるランダムネスの効果

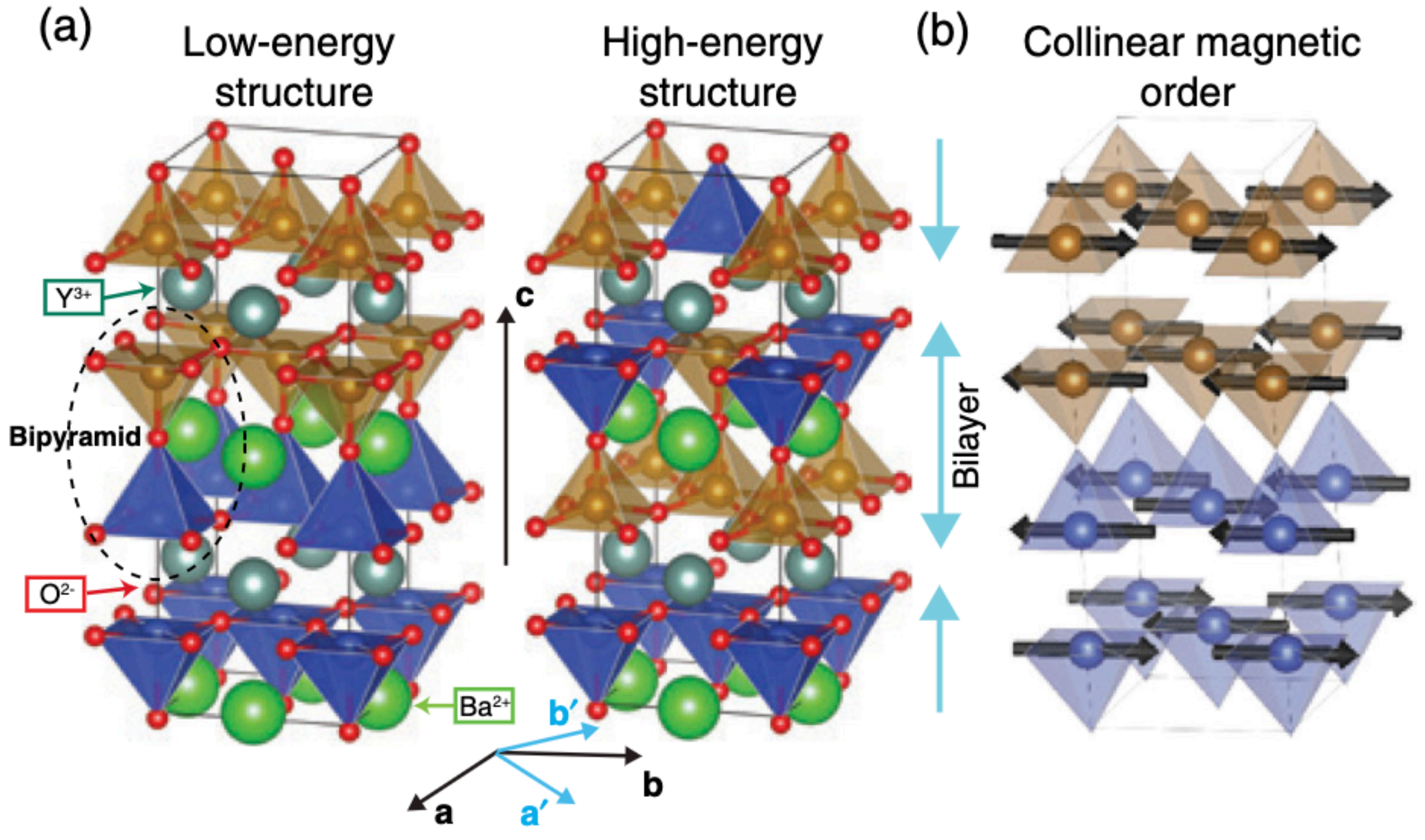



**HS** and M. Imada, PRL **102**, 016404 (2009)

## 磁性体＋ランダムネス

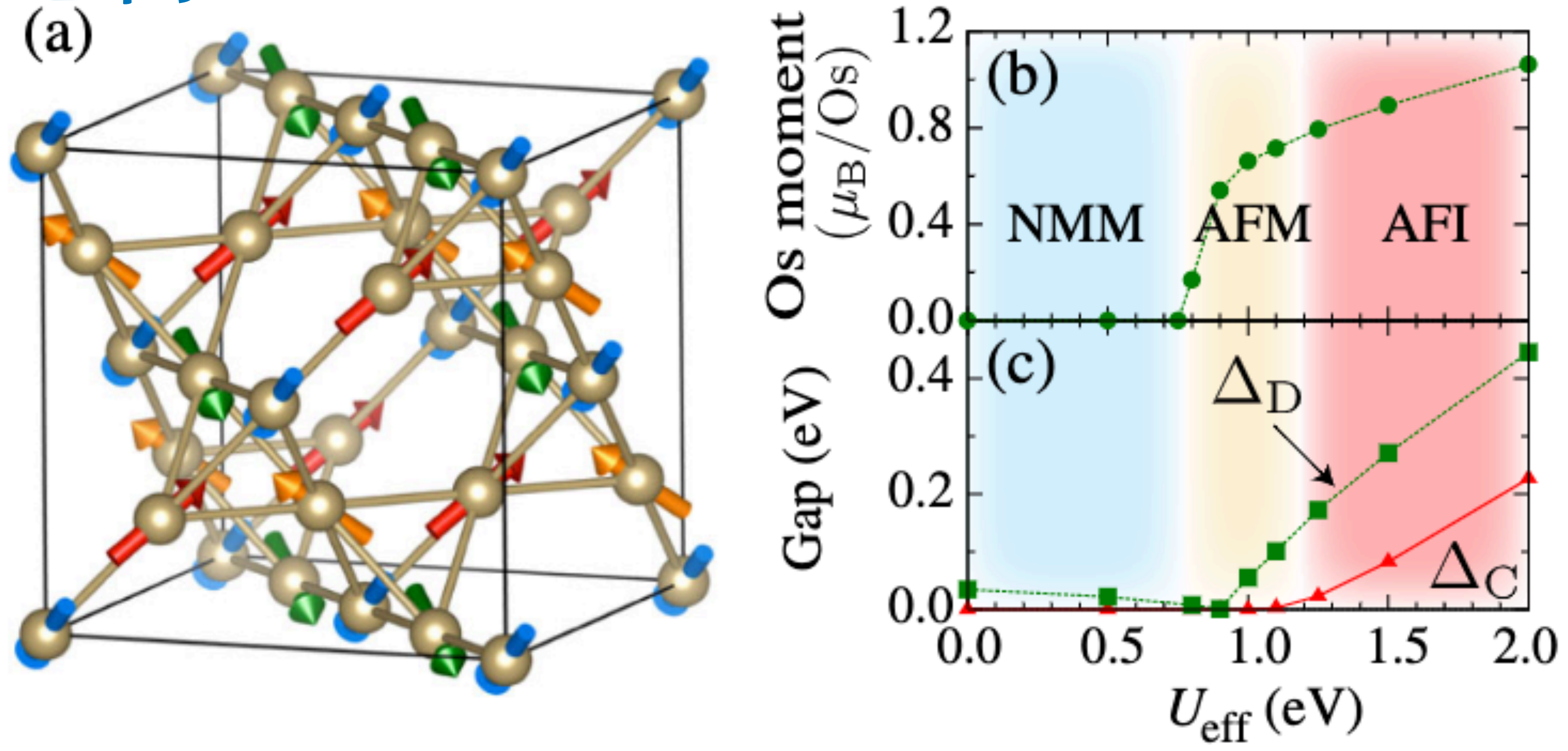



**HS**, Y. Tomita, and Y. Motome, PRL **107**, 047204 (2011)

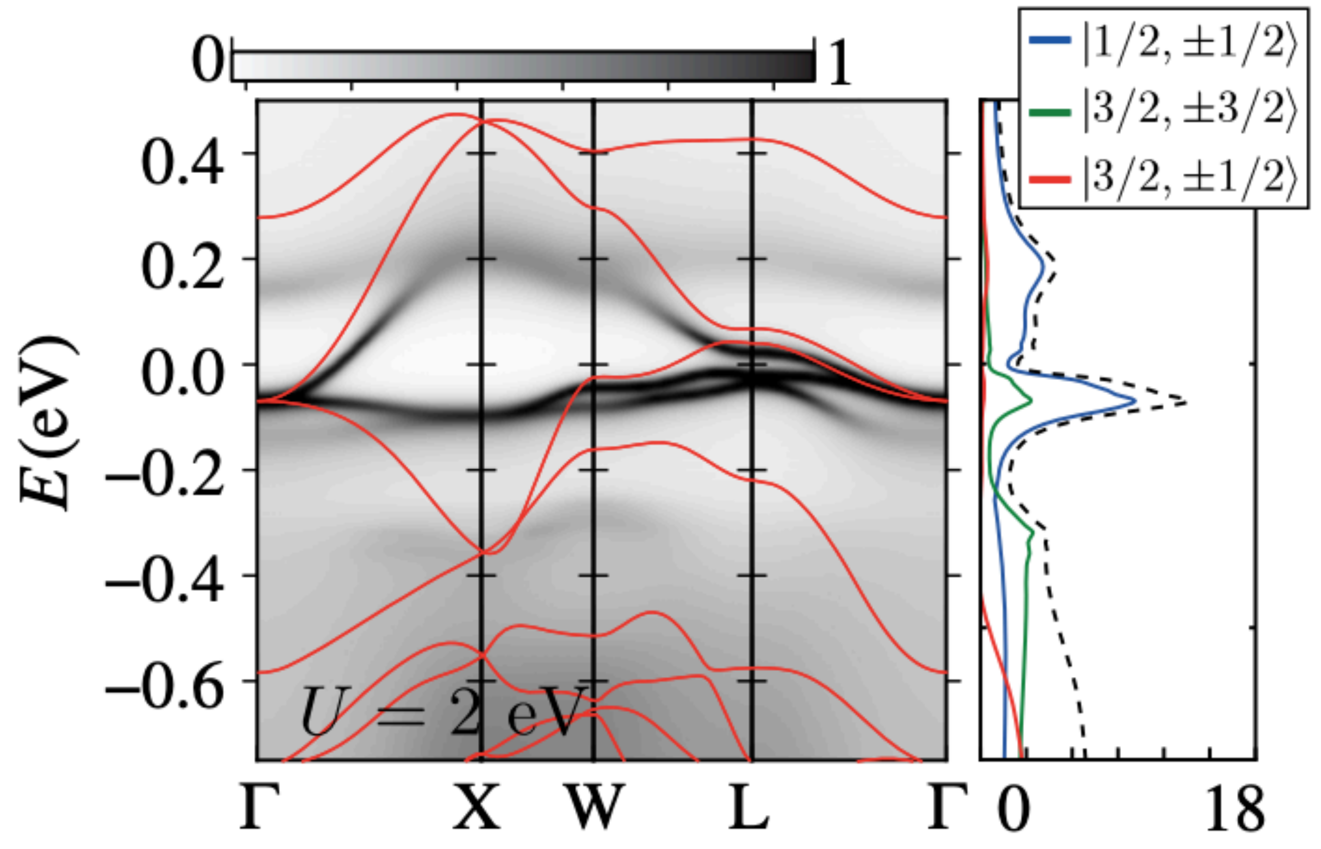



A. Scaramucci, **HS** *et al.*, PRX **8**, 011005 (2018)

## スピン軌道物理




$Cd_2Os_2O_7$: **HS**, T. Miyake, and S. Ishibashi, PRL **108**, 247204 (2012)




Mott physics in $Y_2Ir_2O_7$: **HS**, S. Hoshino *et al.*, PRL **115**, 156401 (2015)



arXiv:2210.12984, arXiv:2303.11819

# Introduction

(強相関電子系を含む)固体の第一原理計算手法を確立したい

## 量子多体理論

動的平均場理論、量子モンテカルロ法、ダウンフォールディング

**HS**, M. Troyer, and P. Werner, PRB **91**, 245156 (2015), C. Honerkamp, **HS** *et al.*, PRB **98**, 235151 (2018), **HS** *et al.*, PRB **92**, 195126 (2015)

## 古典情報理論

スパースモデリング、テンソルネットワーク

**HS**, J. Otsuki, M. Ohzeki, K. Yoshimi, PRB **96**, 035147 (2017)
J. Otsuki, M. Ohzeki, **HS**, K. Yoshimi, PRE **95**, 061302(R) (2017)

## オープンソースソフトウェア開発

DCore, sparse-ir

https://github.com/SpM-lab/sparse-ir

## 量子計算

VQE/VQS

R. Sakurai, W. Mizukami, and **HS**, PRR **4**, 023219 (2022)



arXiv:2210.12984, arXiv:2303.11819

# Overview of this talk

- Introduction
- Multi-scale space-time ansatz based on Quantics tensor trains

  Separation of length scales
- Compression

  From non-equilibrium to equilibrium
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  - Fourier transform, multiplication
  - Dyson/Bethe-Sapleter equation
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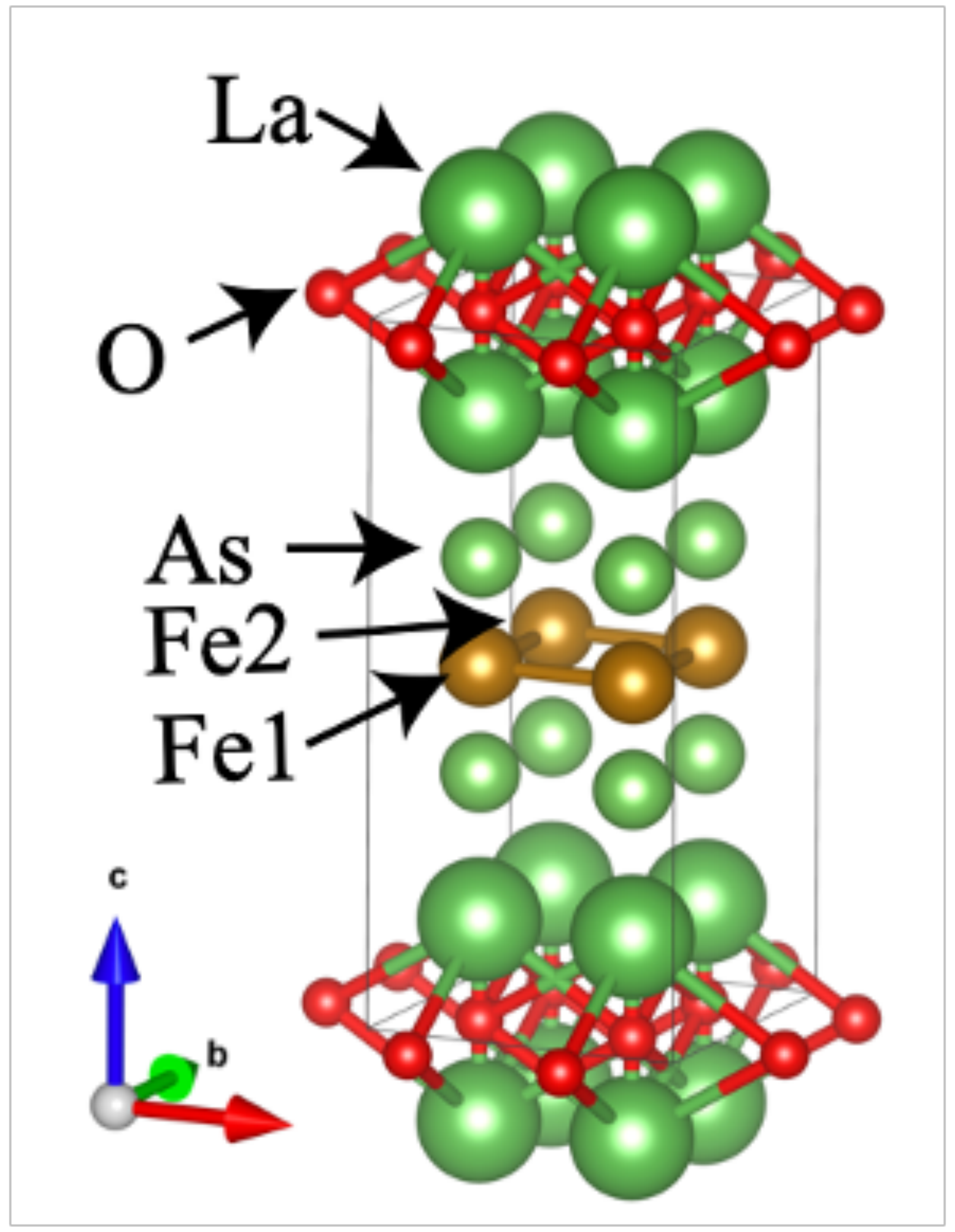
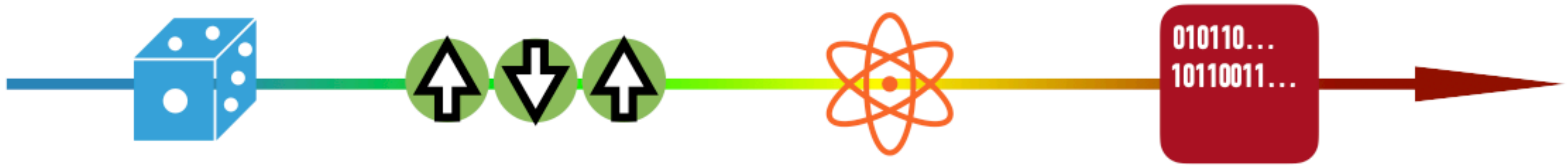
# Where are “solids”?

Many active degrees of freedom
- Long-range Coulomb interactions
- Low-energy excitations

? ?




| Problems | Random Circuit | Cond-mat Physics | Quantum Chemistry | Factoring |
|---|---|---|---|---|

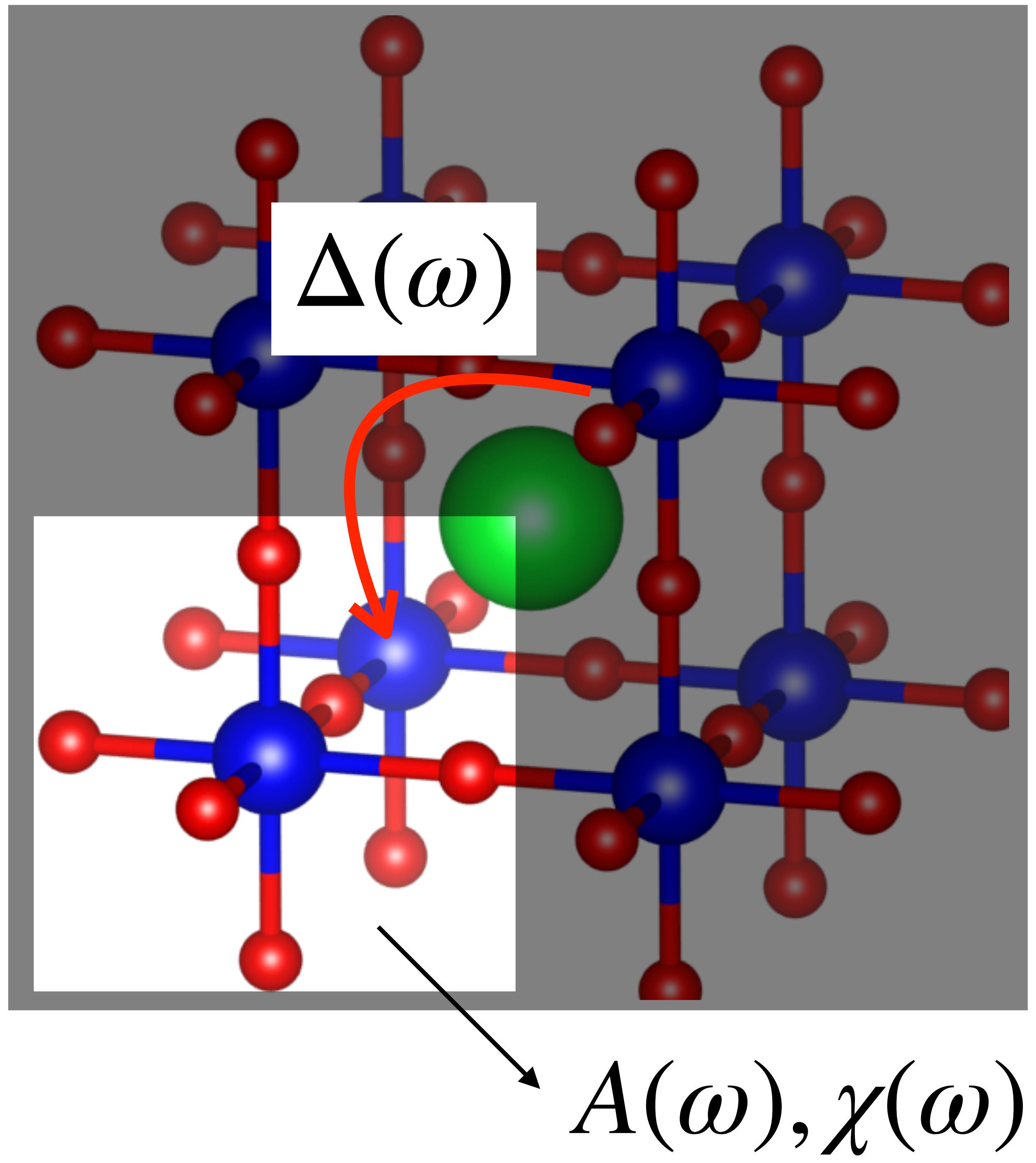



| | | | | |
|---|---|---|---|---|
| #Qubits | $O(10^4)$ | $O(10^5)$ | $O(10^6)$ | $O(10^7)$ |
| Runtime | $O$(Hours) | $O$(Hours) | $O$(Days) | $O$(Days) |

N. Yoshioka, T. Okubo, Y. Suzuki, Y. Koizumi, W. Mizukami, arXiv:2210.14109v1

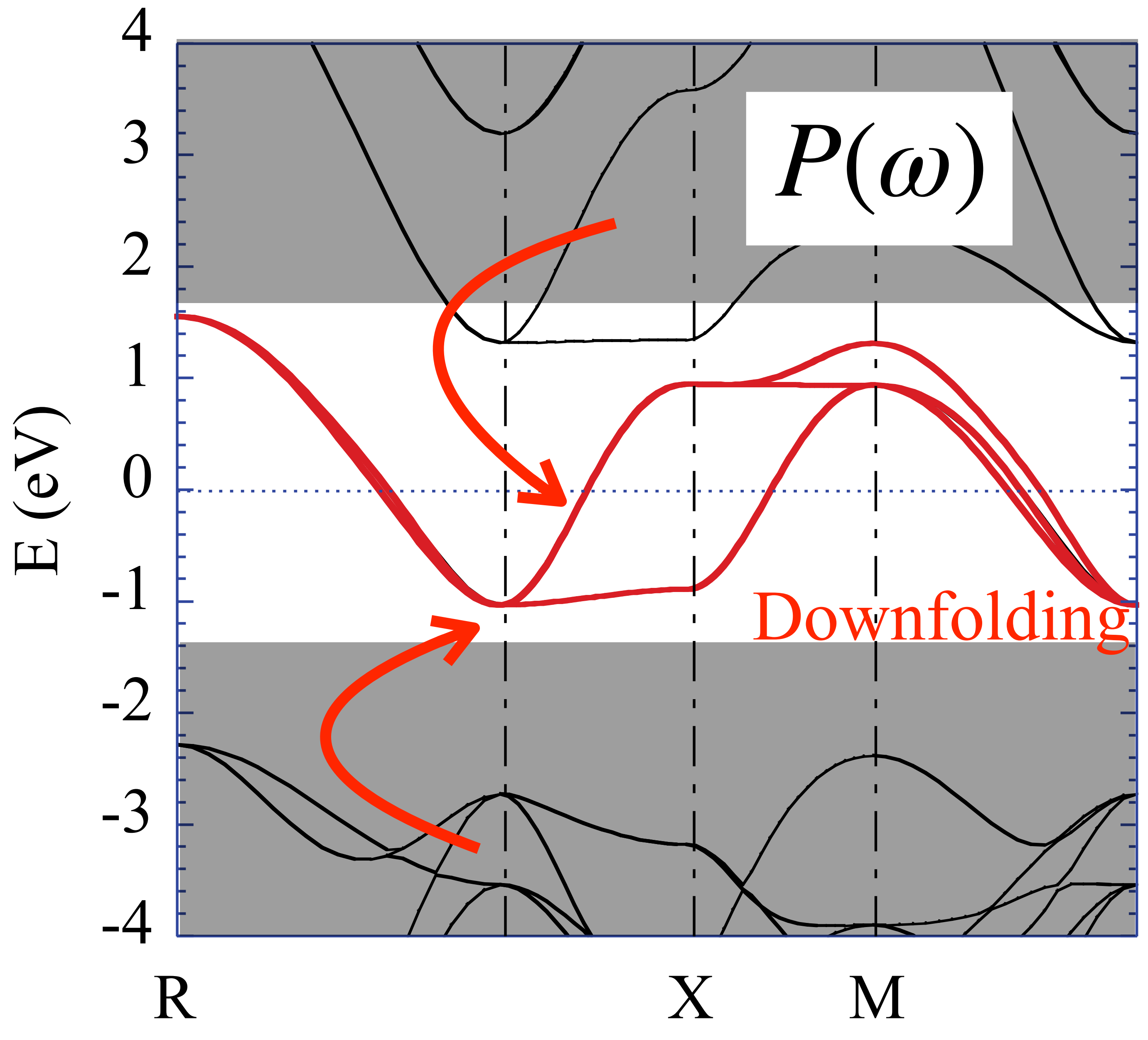
# Connecting different scales

## Embedding in space




Dynamical mean-field theory,
dynamical vertex approximation *etc.*

## Embedding in energy




M. Imada and T. Miyake (2010)

Constrained RPA *etc.*

**Grand challenges**

- More accurate embedding based on *sophisticated* diagrammatic theories
- Efficient treatment of space-time dependence

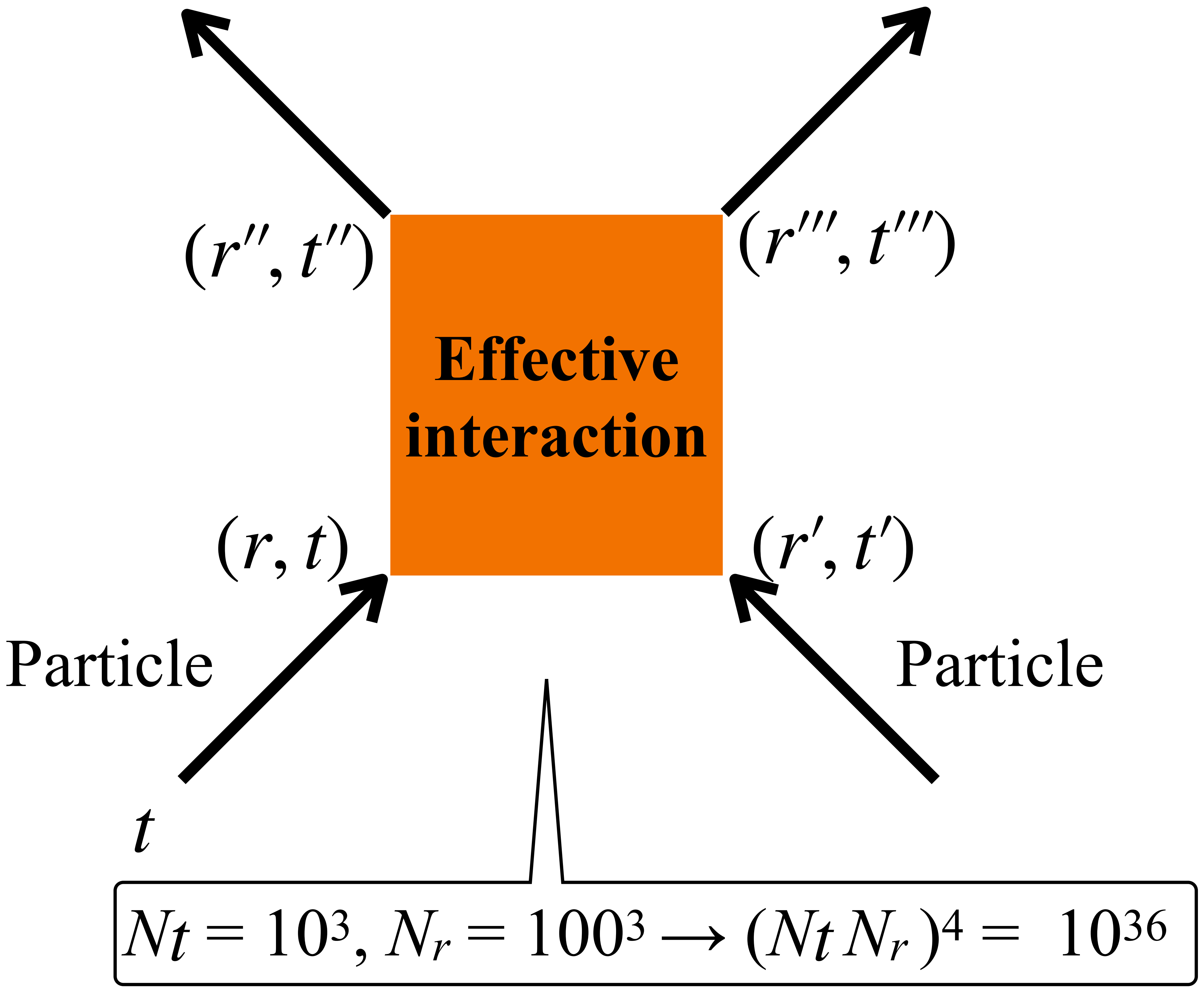
# Correlation functions in a high-dimensional space-time domain

## One-particle (1P) level

Symmetry breaking


## Two-particle (2P) level

Susceptibility, beyond mean field




High demand for efficient numerical treatment

Three dimensional systems, multi-particle level, nonequilibrium systems



arXiv:2210.12984, arXiv:2303.11819

# 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)
- Minimax 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)



arXiv:2210.12984, 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.

# What we need

- Accurate treatment of a wide range of length scales in space-time
- Systematic control over truncation error
- Efficient computations in compressed form
- Straightforward and robust implementations as computer code

Answer: Multiscale space-time ansatz based on quantics tensor trains

HS, M. Wallerberger, Y. Murakami, K. Nogaki, R. Sakurai, P. Werner, A. Kauch, arXiv:2210.12984v2 (to appear in PRX)
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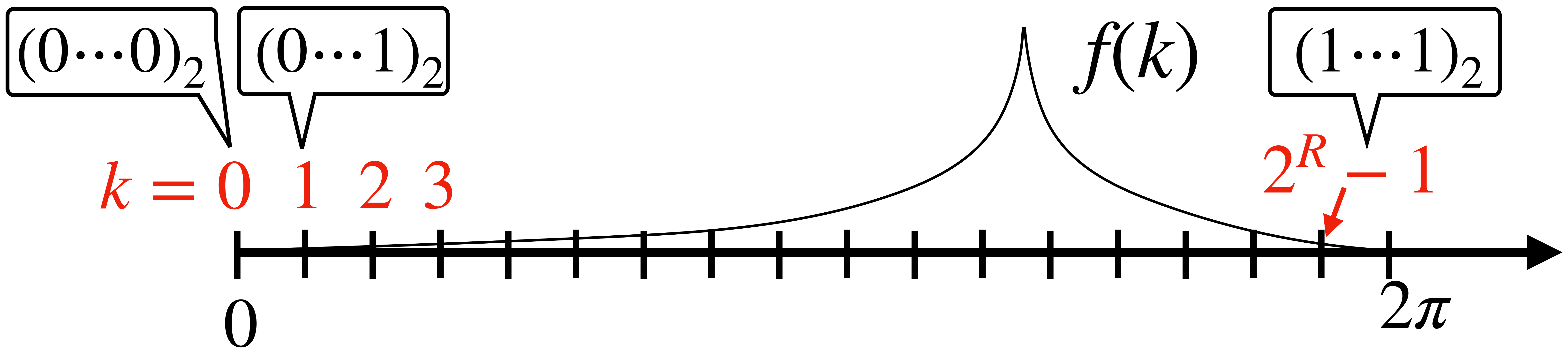
# Quantics tensor train (QTT)

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



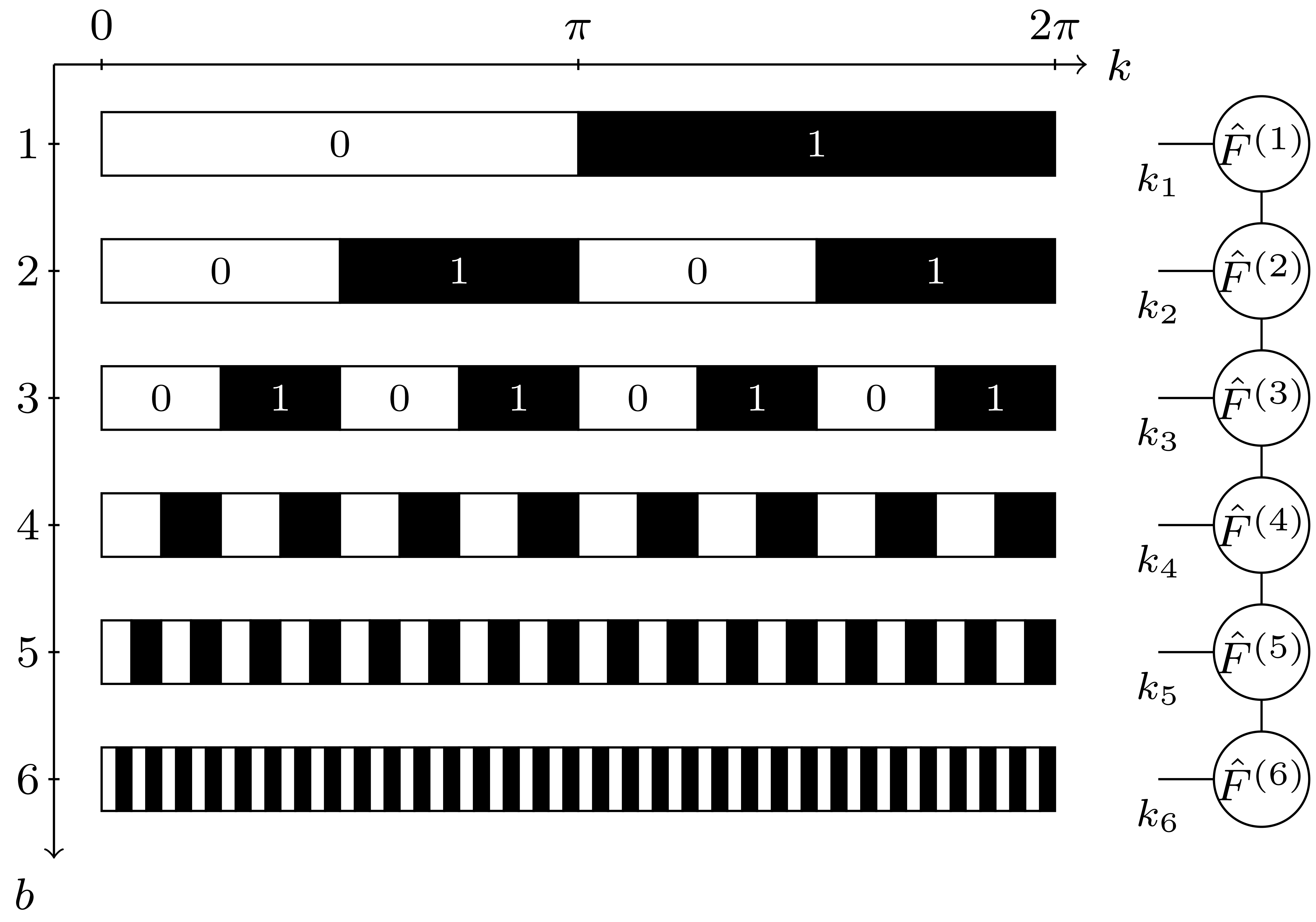

$k = (k_1 \cdots k_{R-1} k_R)_2$

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

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

Tensor train/Matrix product state

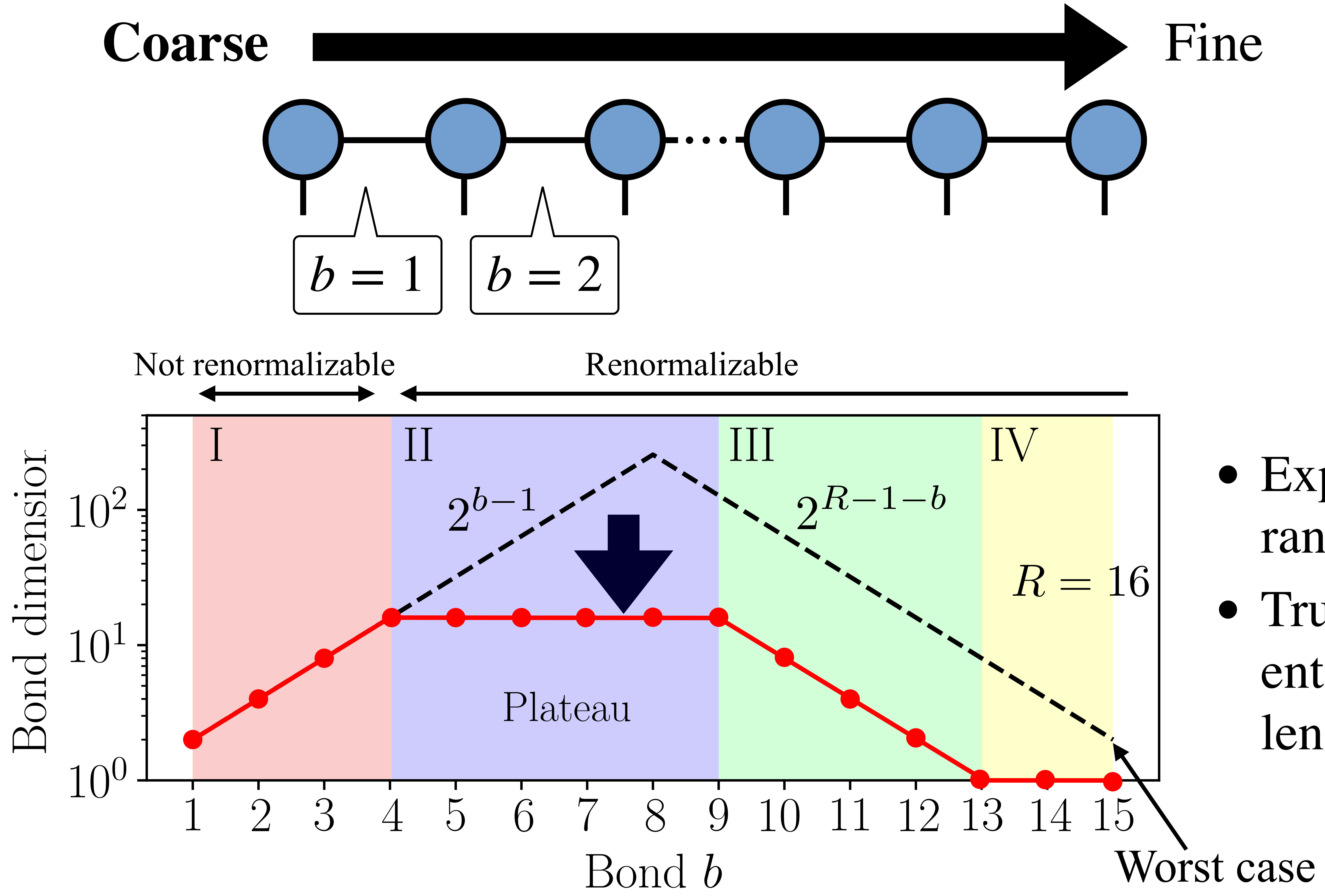
Exponential advantage for storage!






arXiv:2210.12984, arXiv:2303.11819

# Length-scale separation



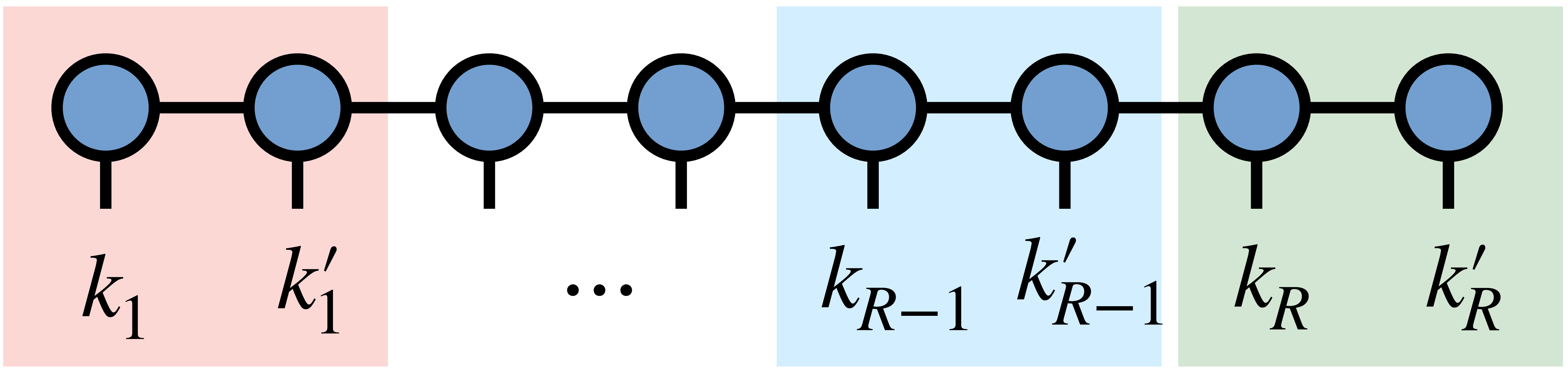

- Exponentially wide range of length scales
- Truncation limits entanglement between length scales.



arXiv:2210.12984, arXiv:2303.11819

# Quantics tensor train (QTT)

## Multivariate function $f(k, k')$



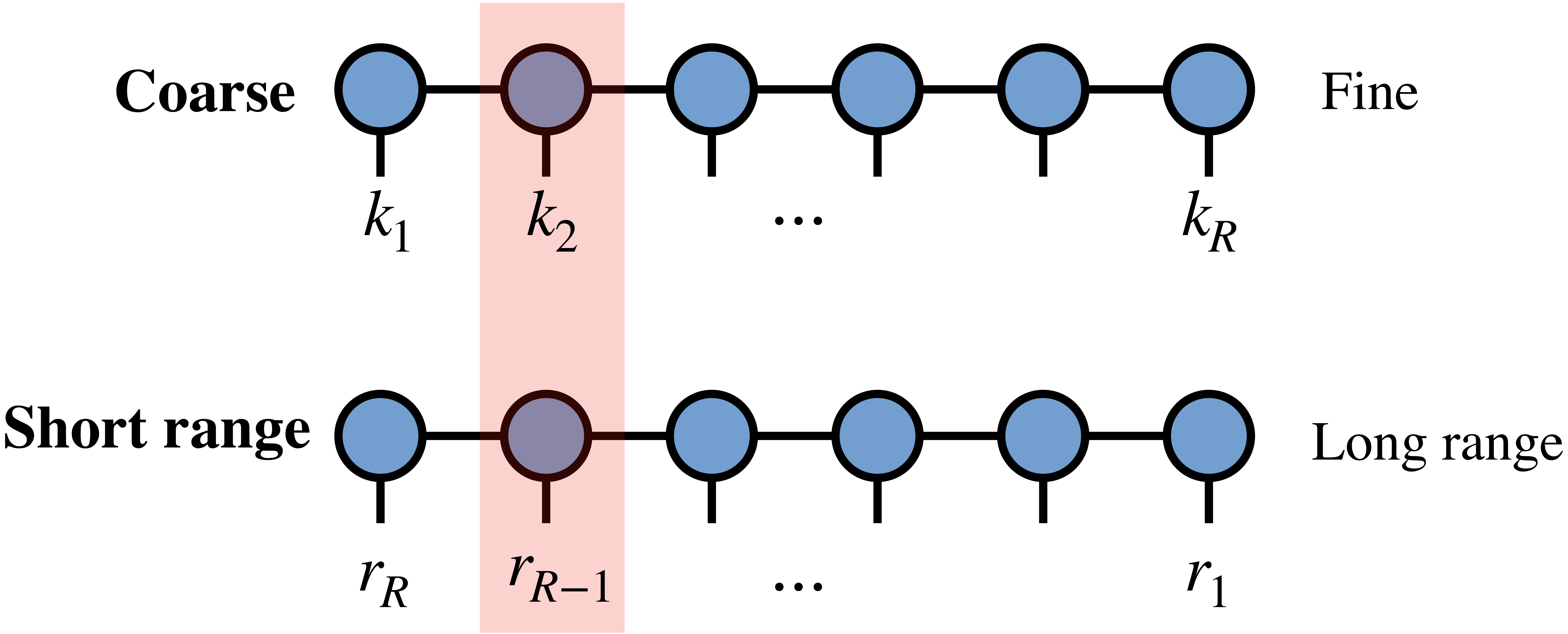

Same length scale

## Fourier transform

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

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

$$r = 0, 1, \cdots, 2^R - 1$$




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



arXiv:2210.12984, arXiv:2303.11819

# Simple examples

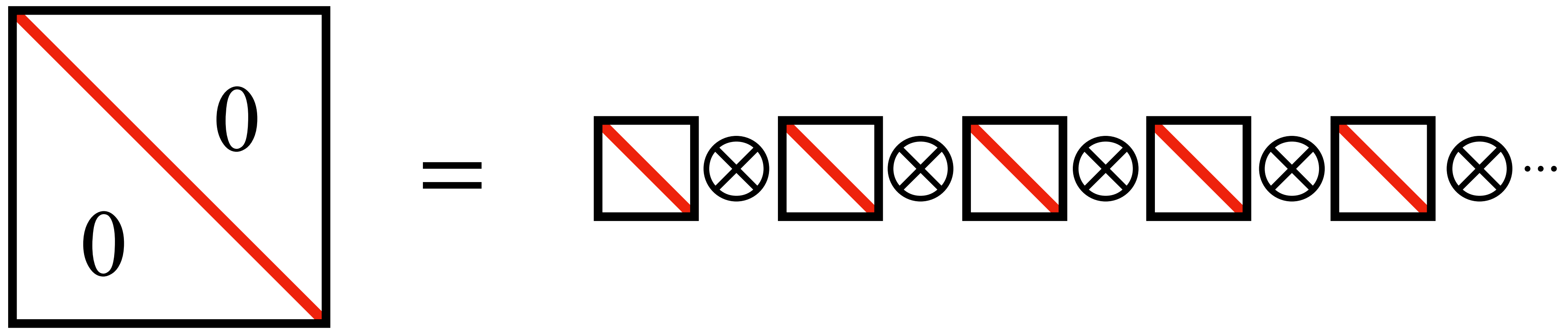
## Exponential function

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

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

## Identity matrix

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






arXiv:2210.12984, arXiv:2303.11819

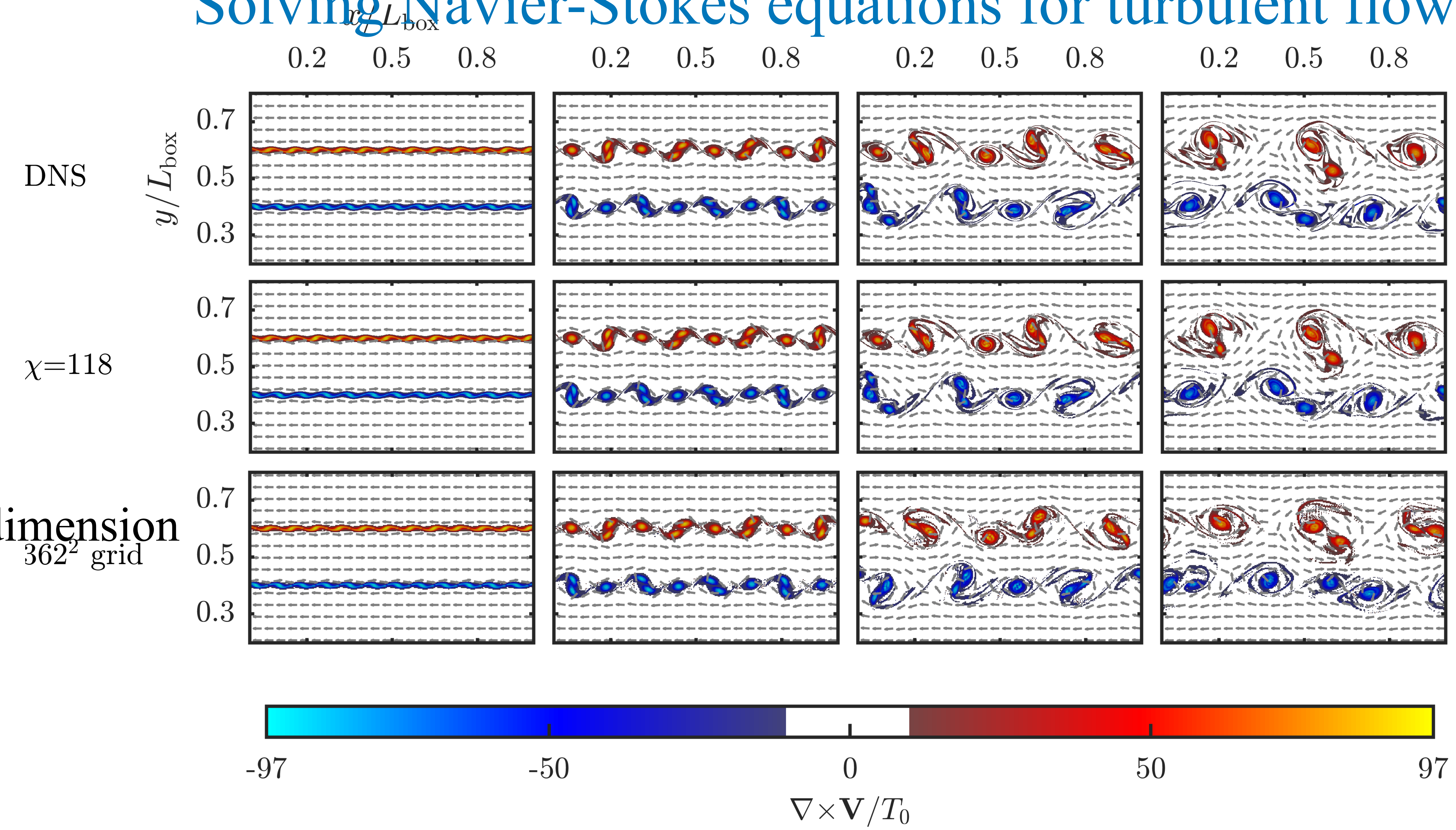
# Recent work on classical systems

## Image compression


Bond dimension

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

## 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?



arXiv:2210.12984, arXiv:2303.11819

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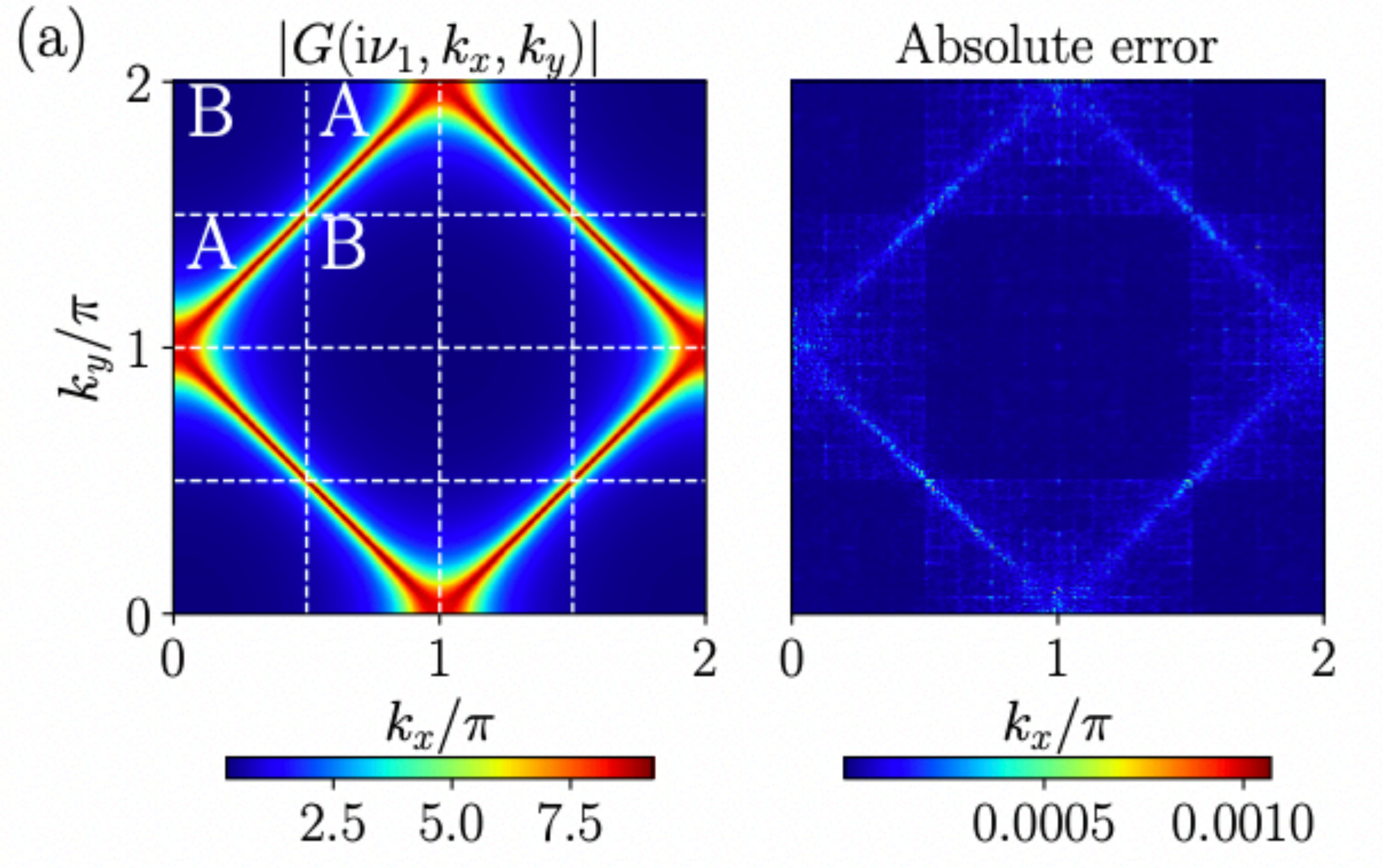
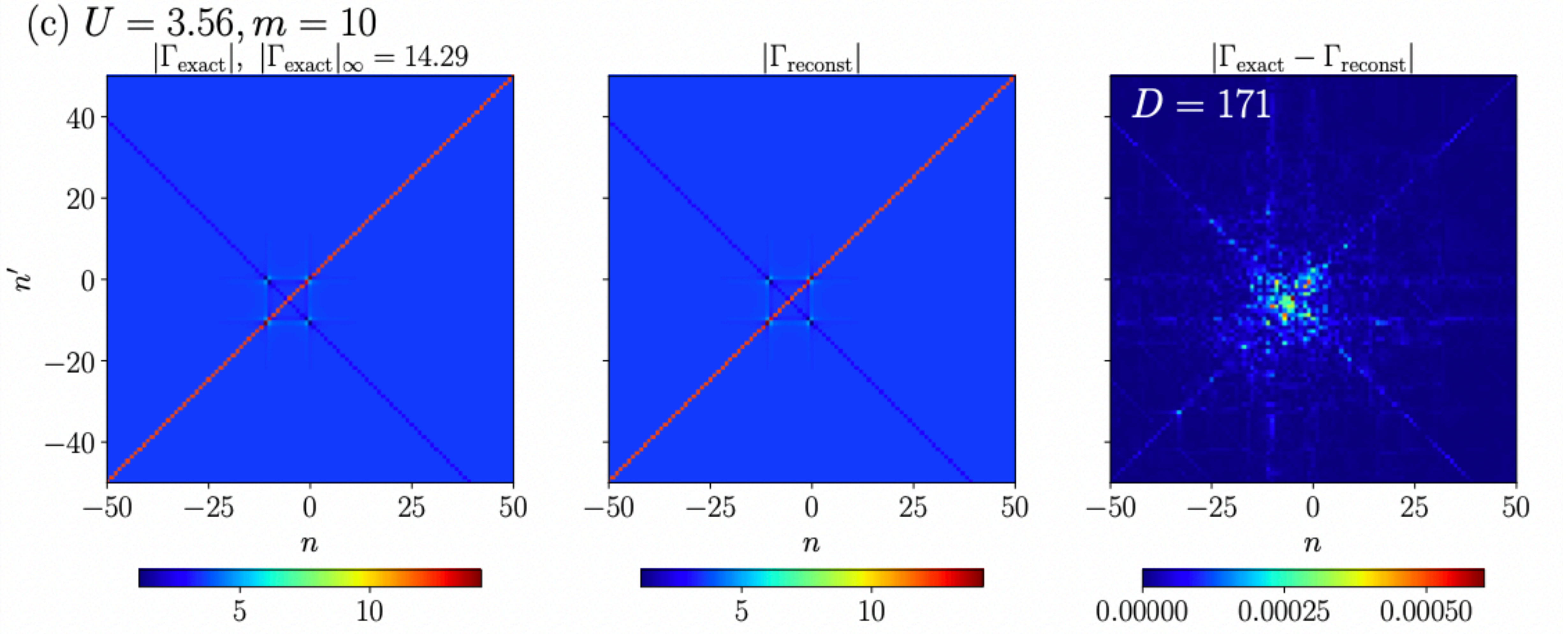
# Compression

## 1P momentum space

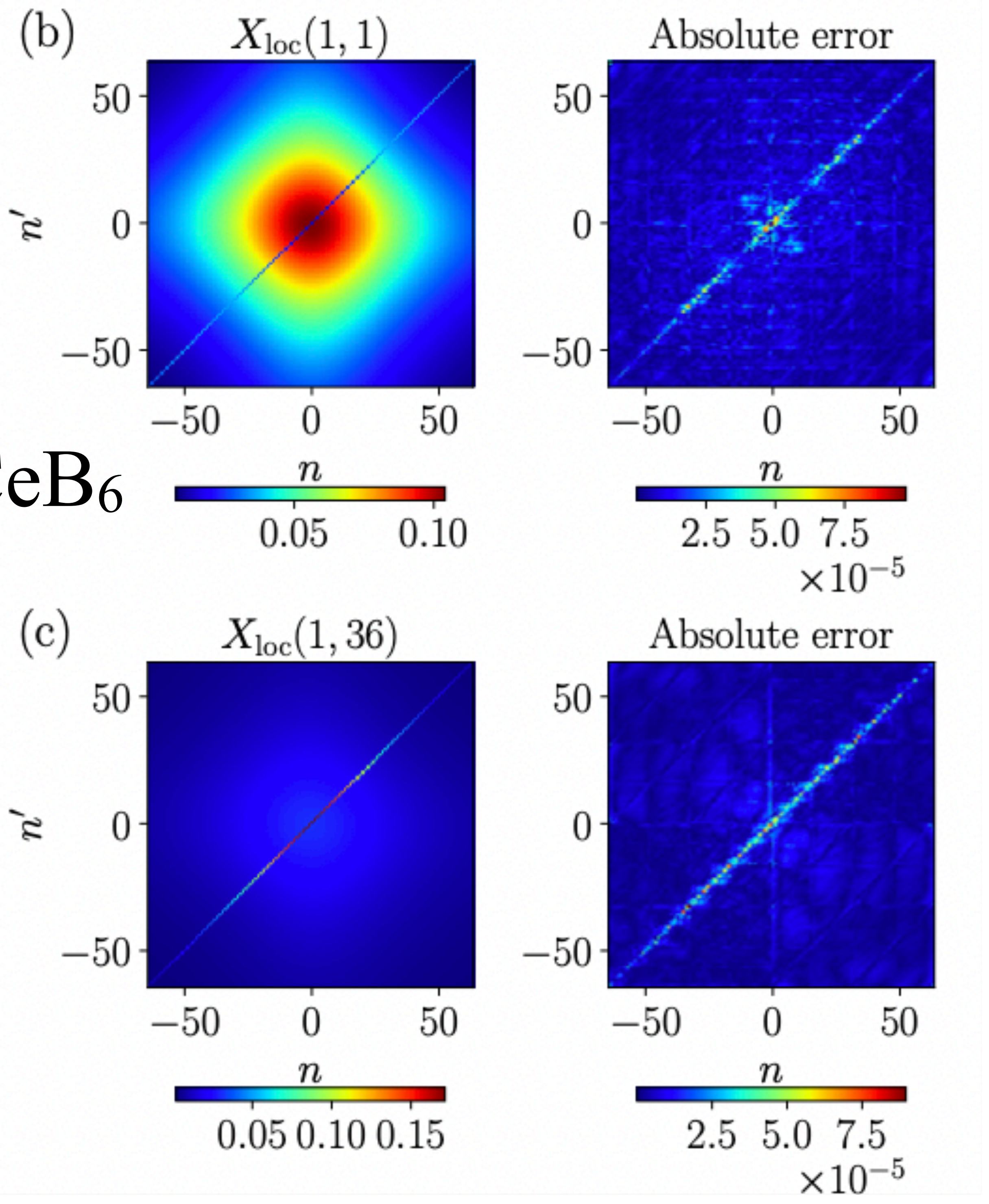



## 2P vertex functions



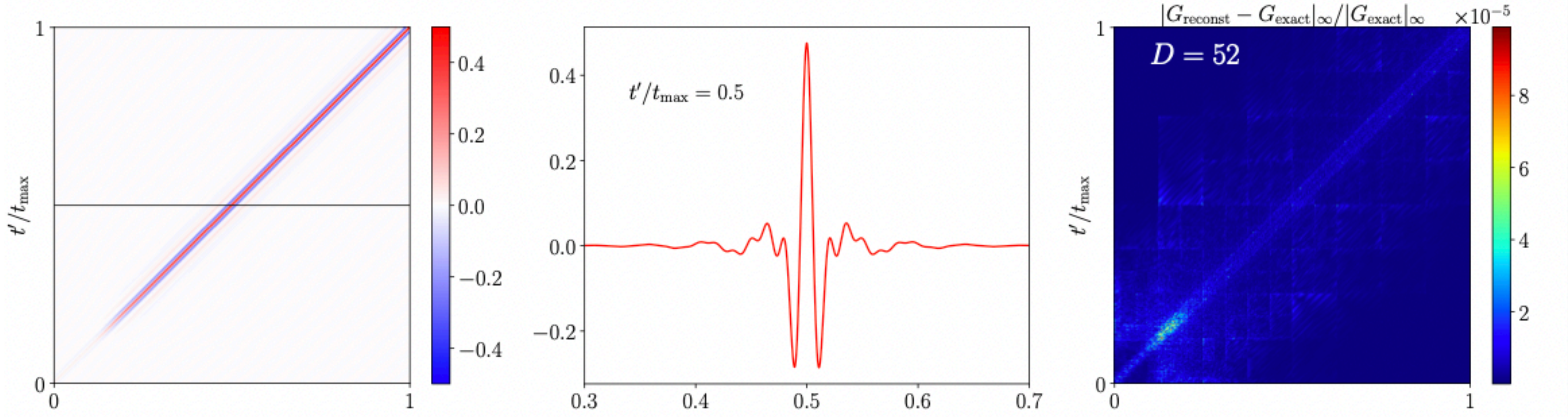

and more

## Multipolar susceptibility




CeB6

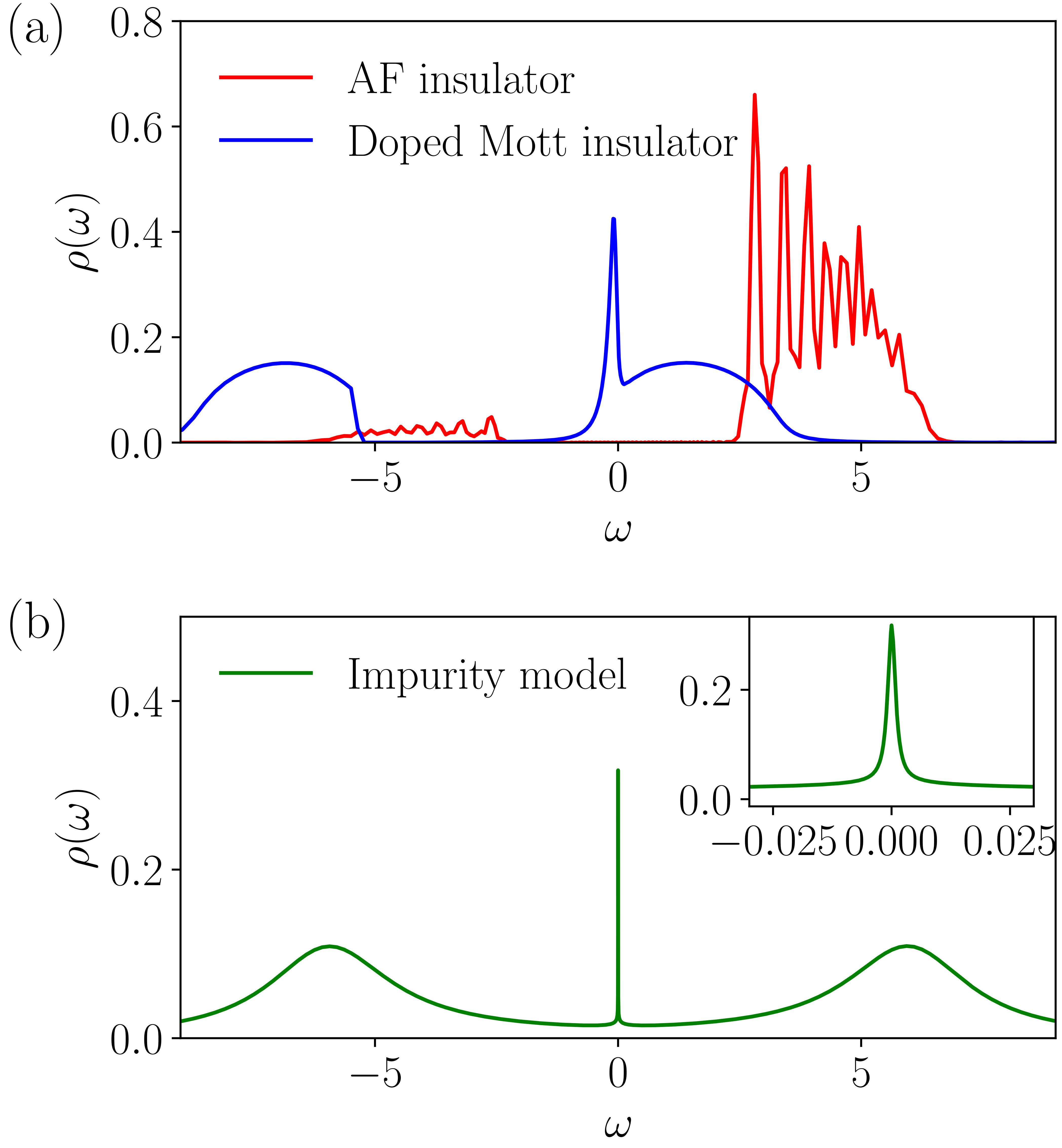
## Nonequilibrium system (real-time Green's function)

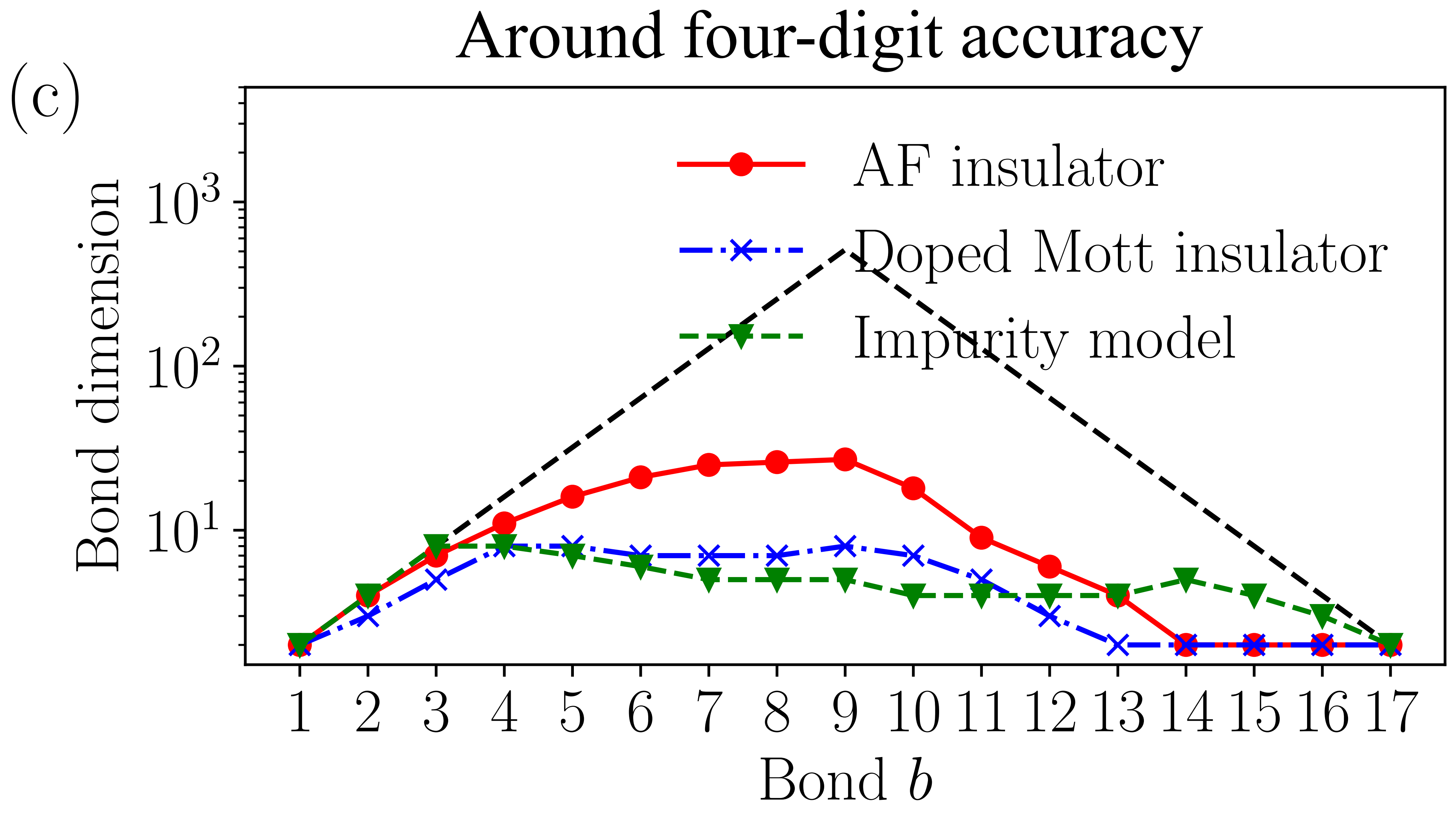





arXiv:

# Spectral functions



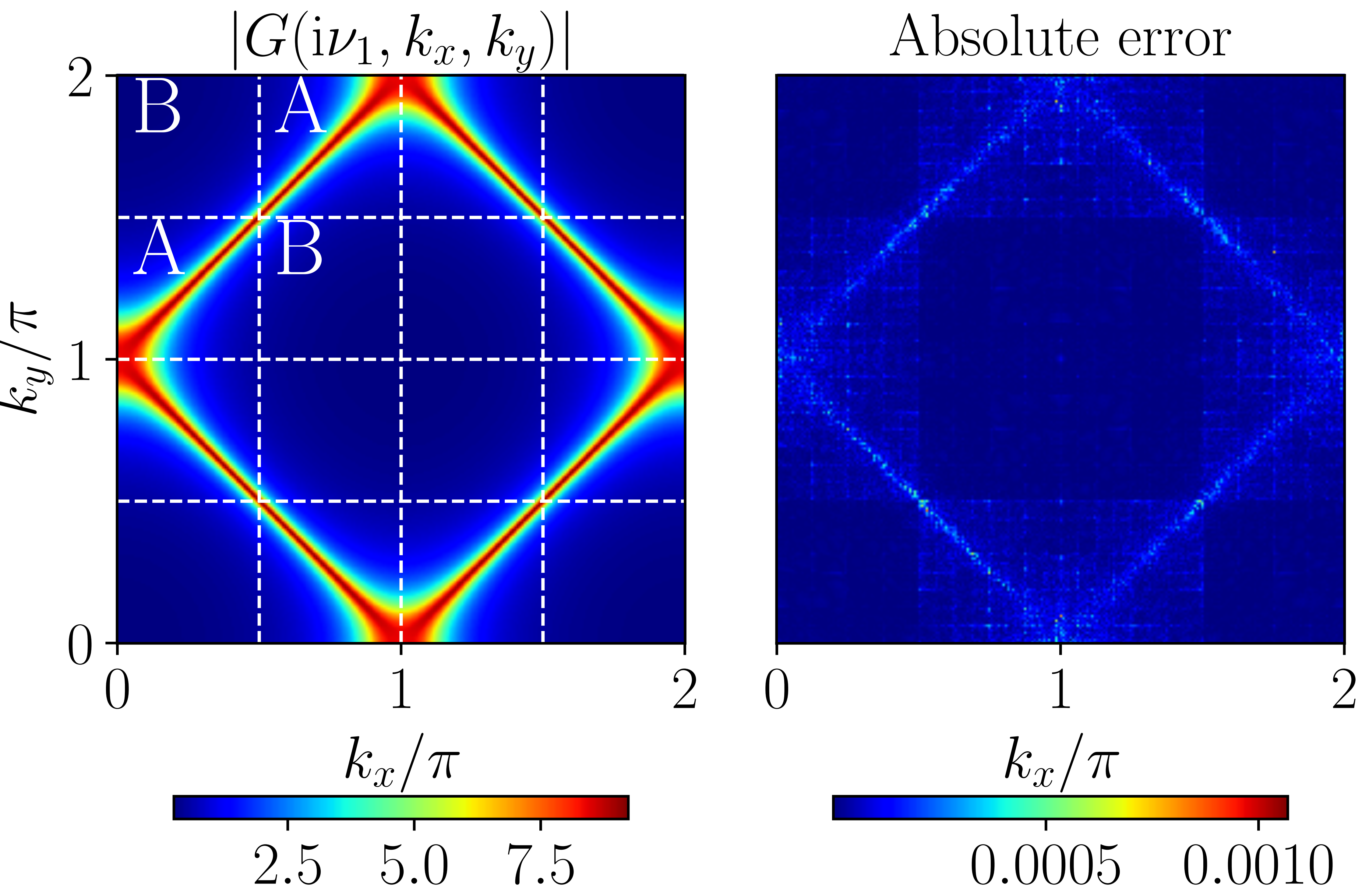

- Sharp peaks can be represented.
- Larger bond dimension for more features

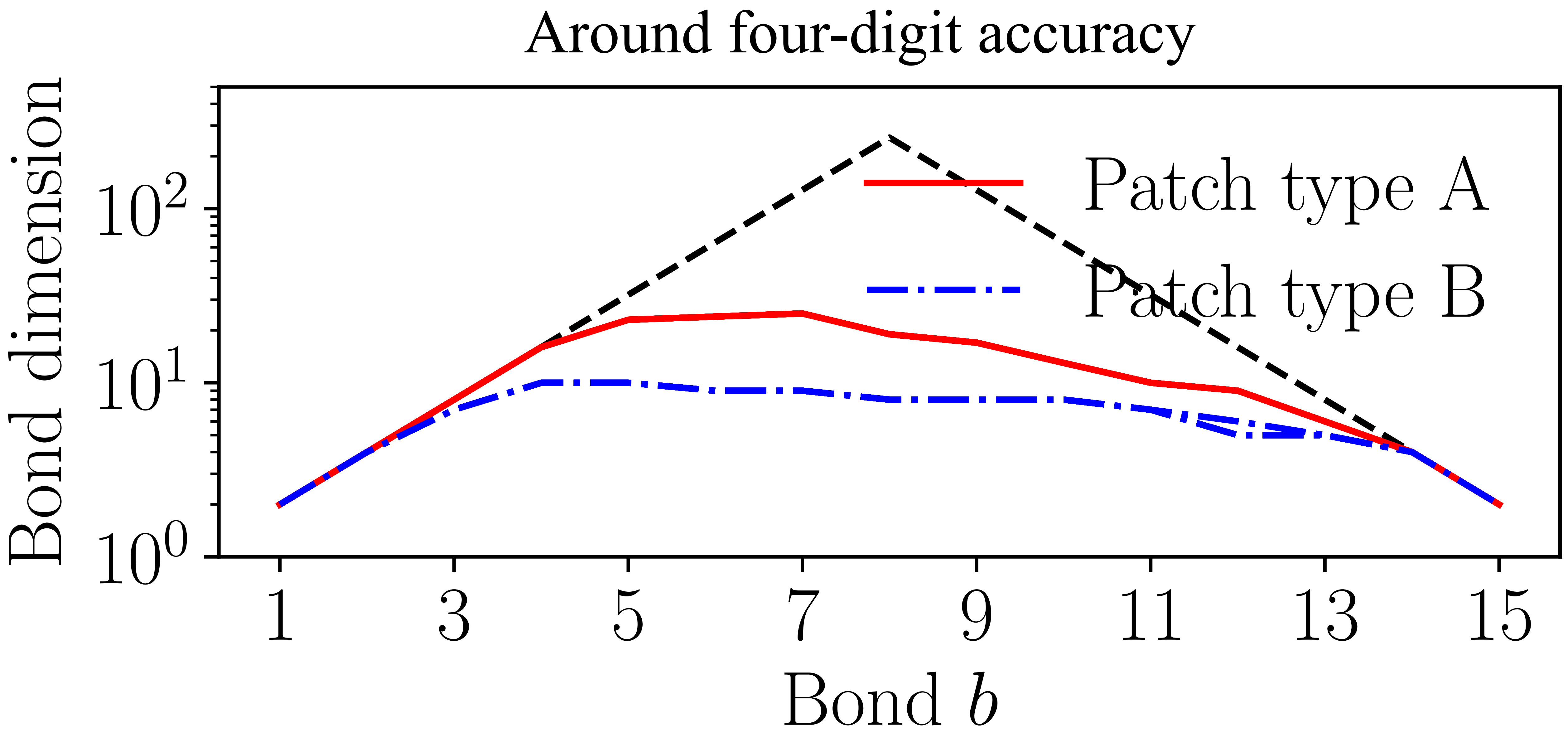


arXiv:2210.12984, arXiv:2303.11819

# Momentum-resolved Green's function

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






arXiv:2210.12984, arXiv:2303.11819

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

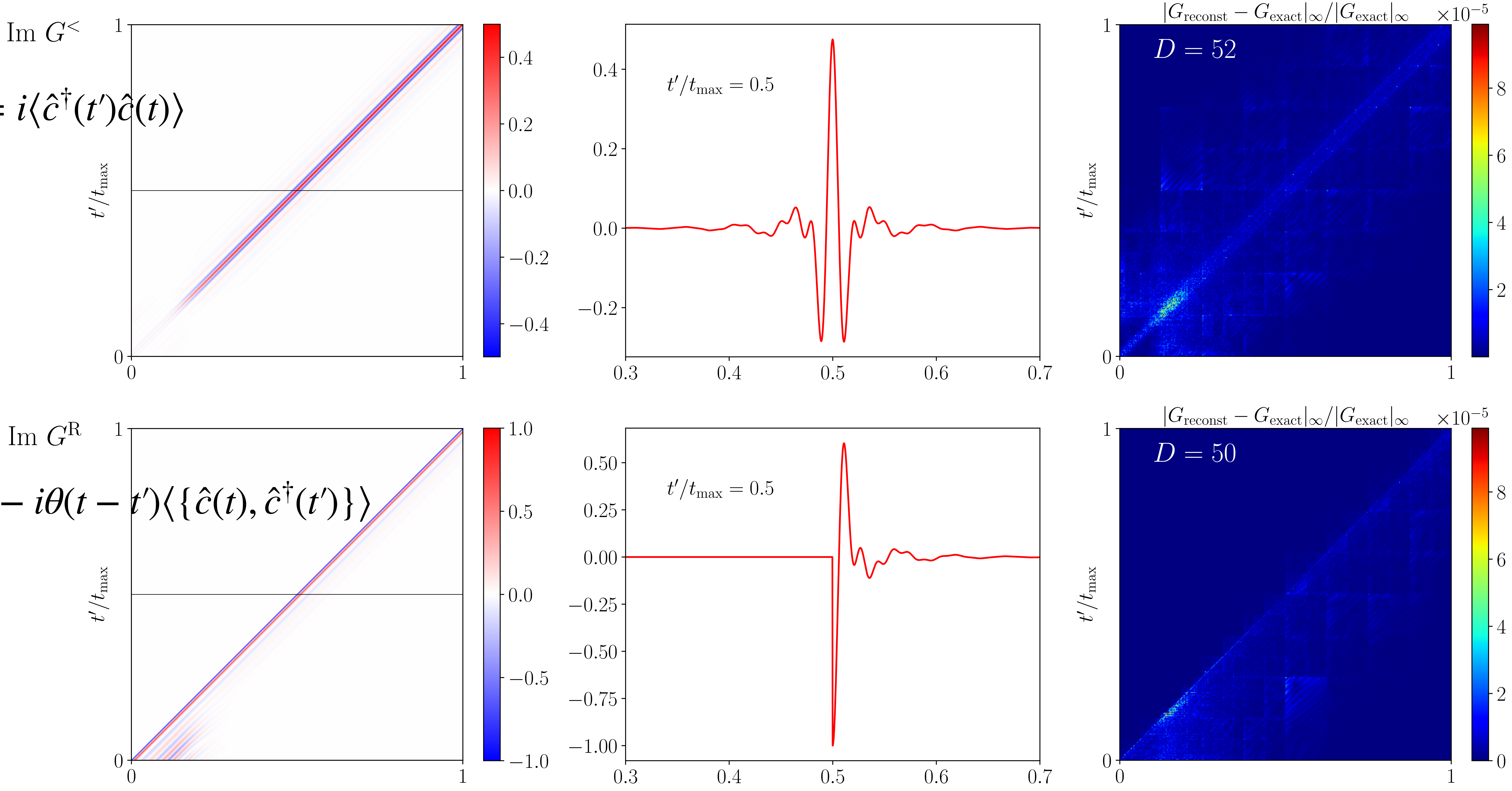
Low-$T$ AF Mott phase excited by a short electric field pulse, Bethe lattice, $T = 0.05$

Compression ratio ~ $10^3$

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

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

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



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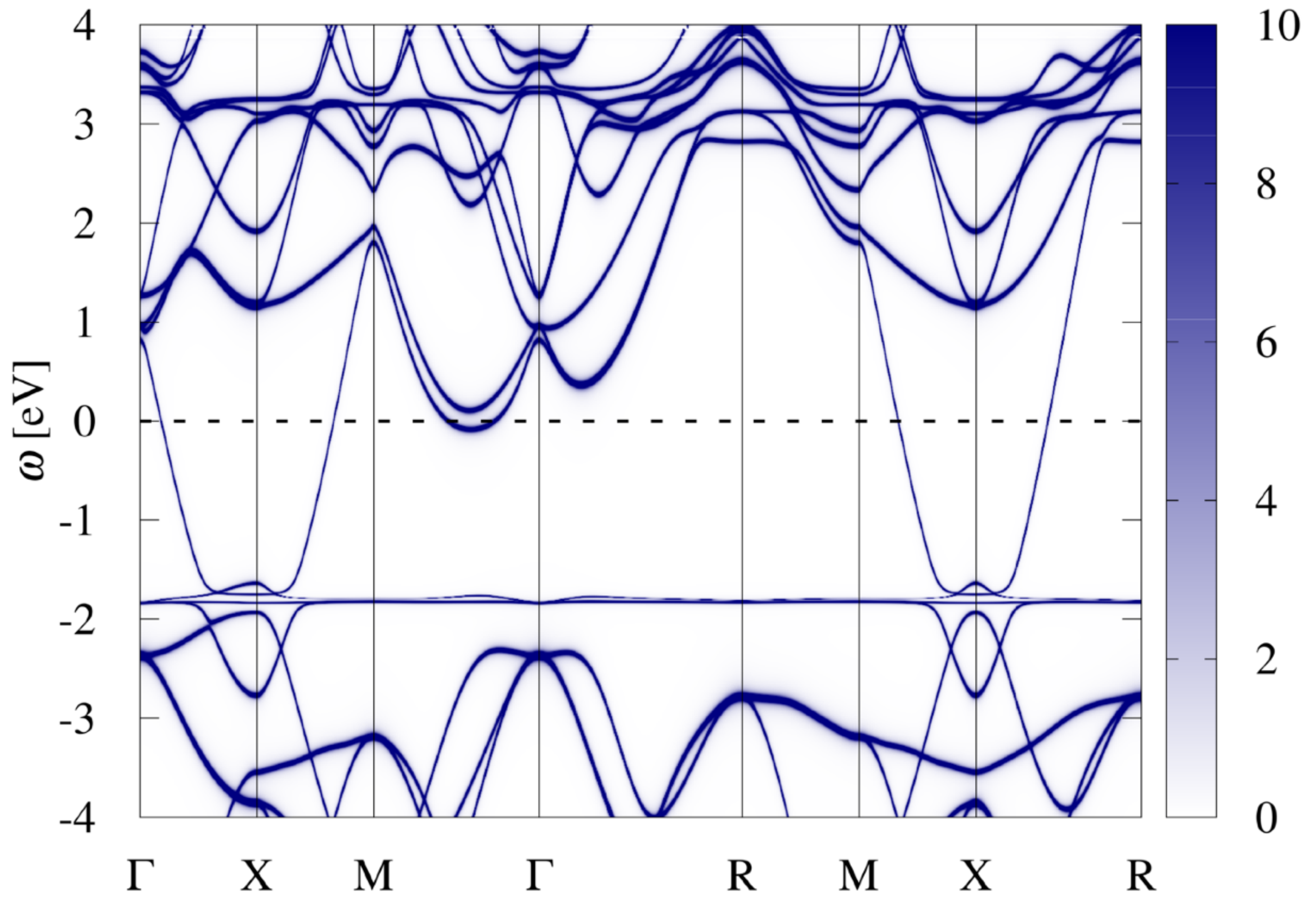
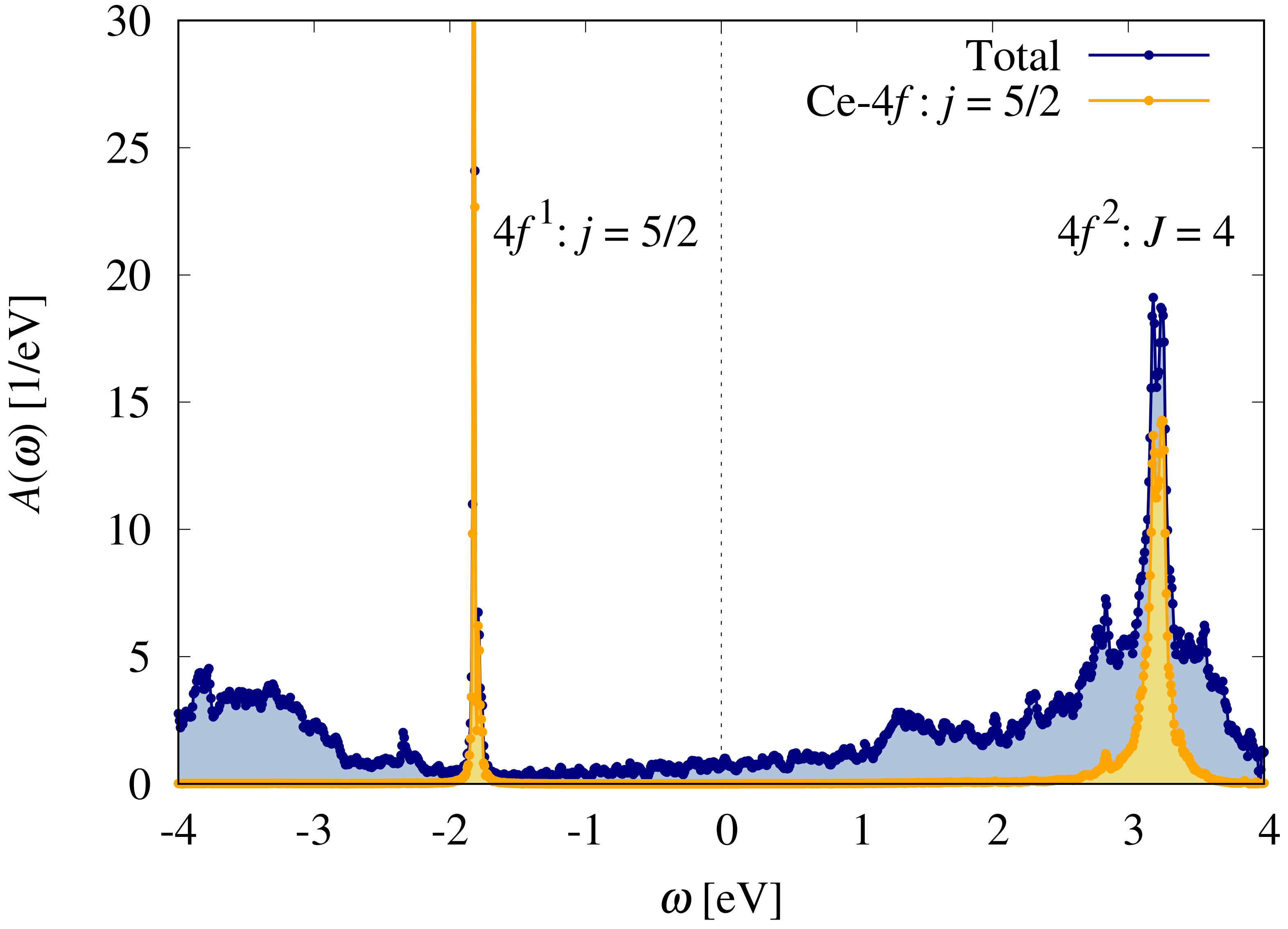
# Multipolar susceptibility of an *f*-electron system: $CeB_6$




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




## Going to analyze high-dimensional data

1. Local generalized susceptibility $N^2 \times N^2 \times N_w \times N_w$

$N = 6,\ N_w = 128(= 2^7)$

2. Multipolar susceptibility $N^2 \times N^2 \times N_q \times N_q \times N_q$

$N_q = 32$

Acknowledgment to J. Otsuki for providing us with huge numerical data



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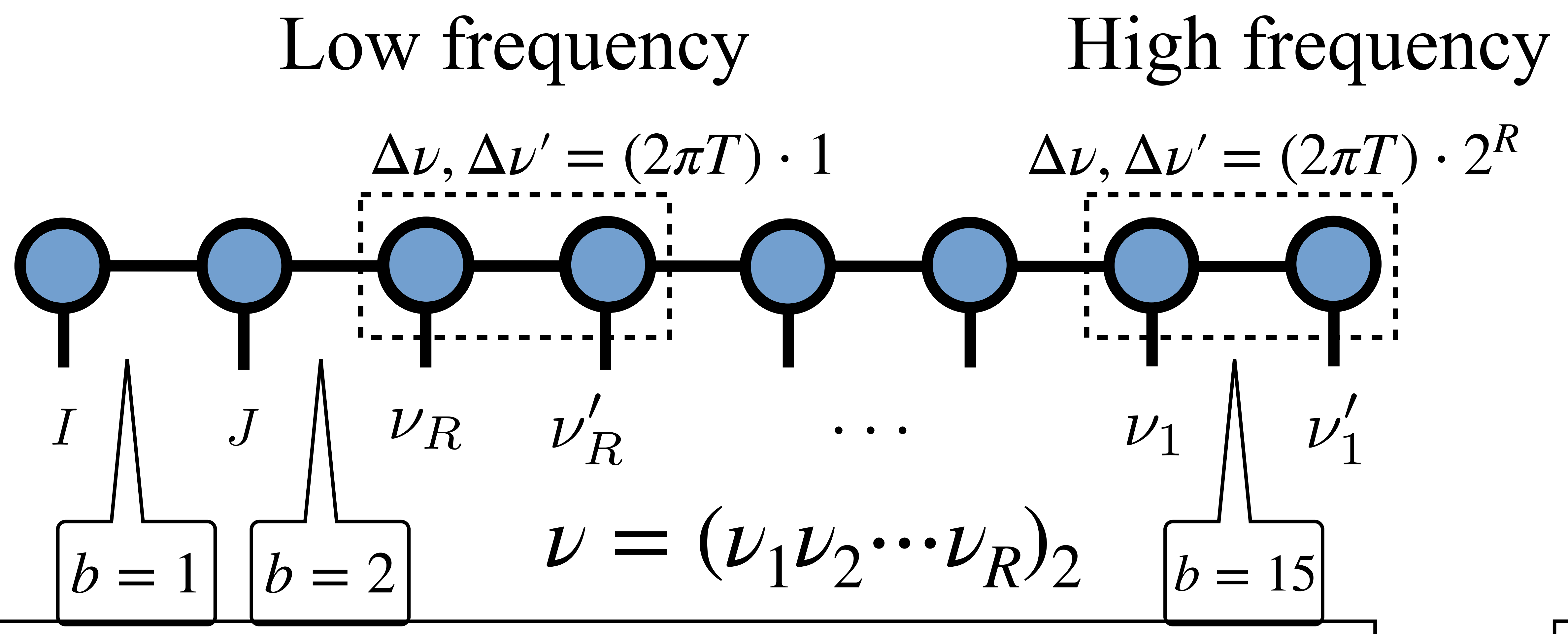
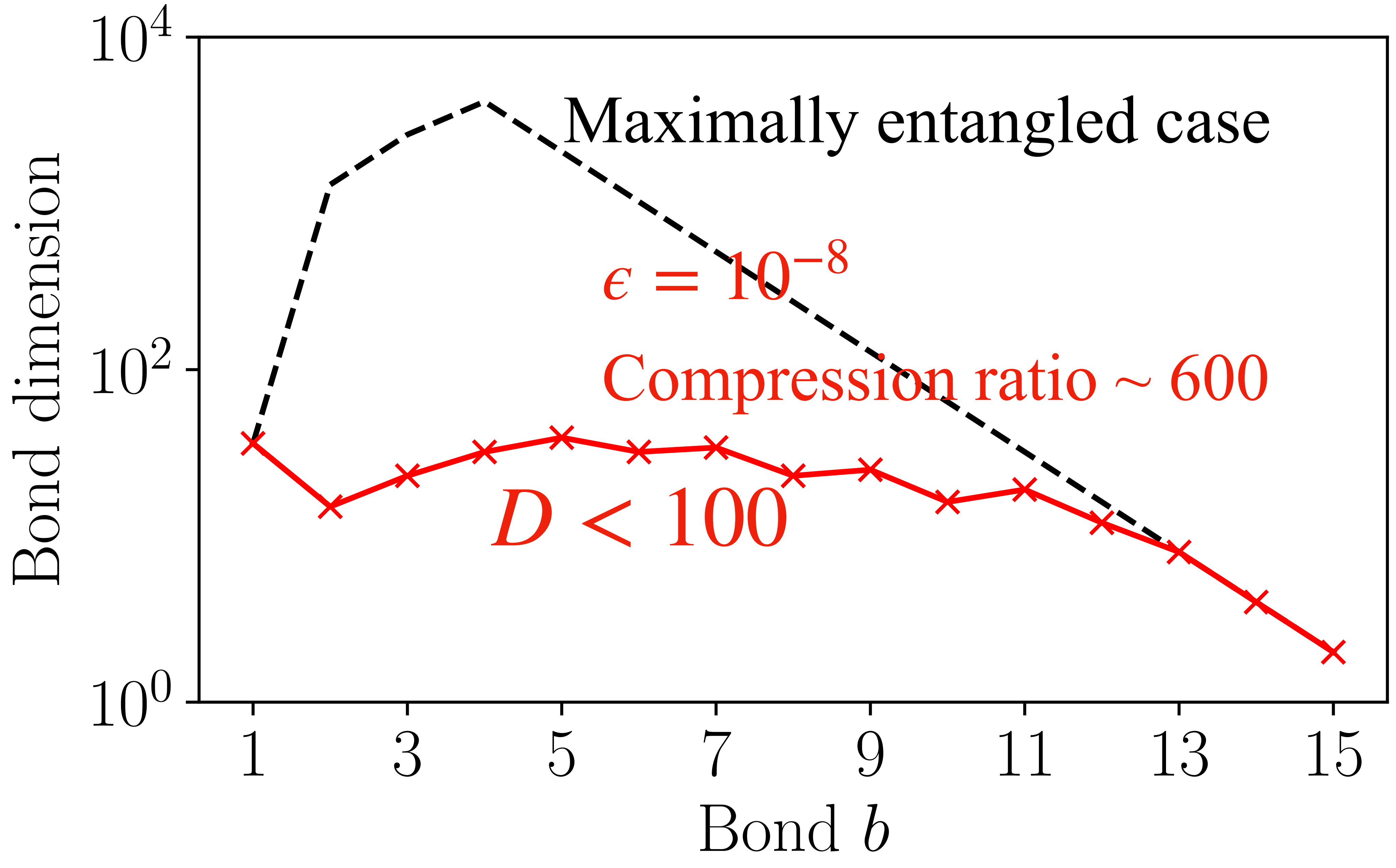
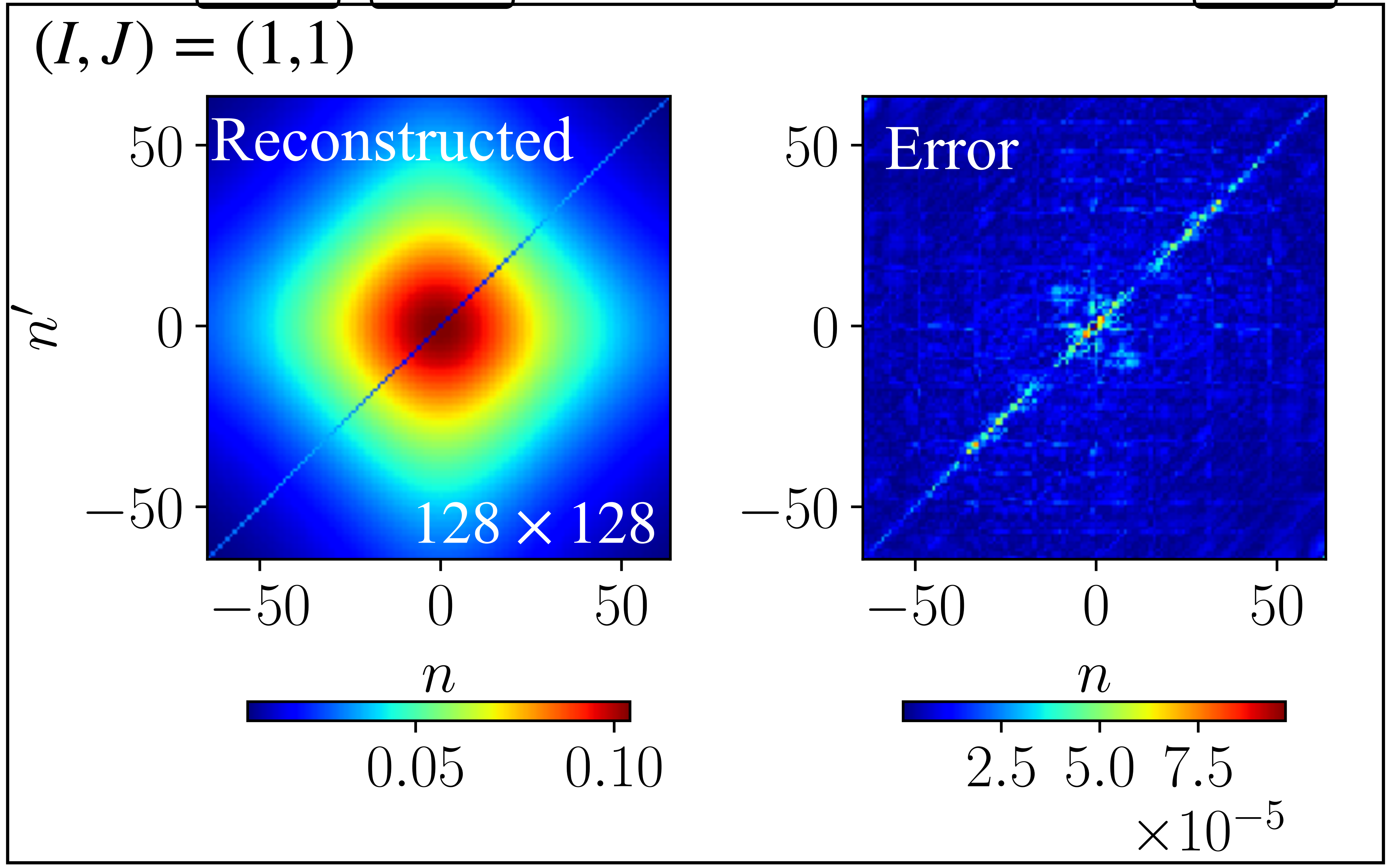
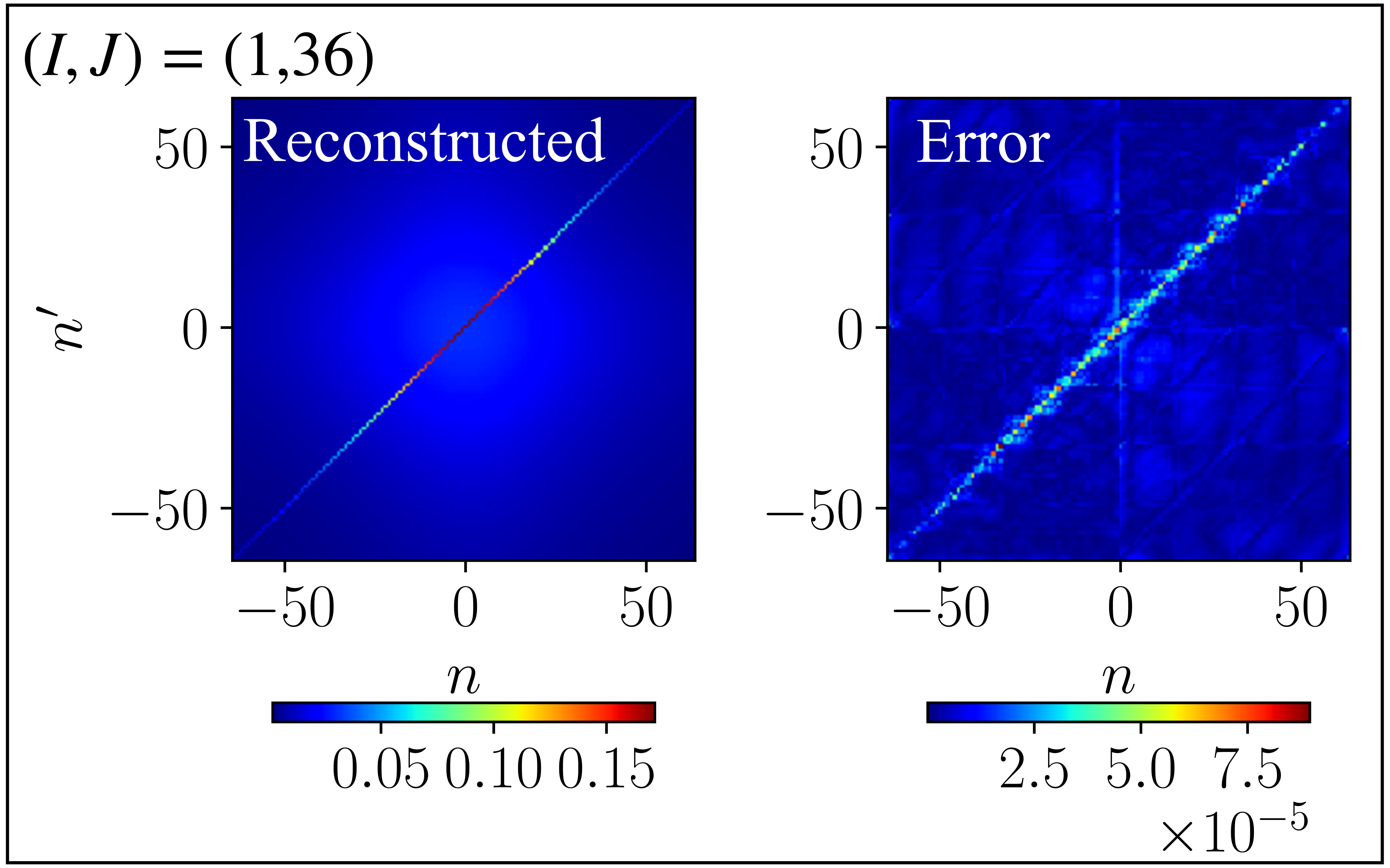
# Local generalized susceptibility






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

arXiv:2210.12984, arXiv:2303.11819

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# Essential operations for diagrammatic calculations

Building blocks of Dyson, Bethe-Salpeter equations *etc*.

1. Fourier transform
2. Element-wise multiplication
3. Convolution

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

$$C(t) = A(t)B(t)$$

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

Mapped to standard MPS calculations using *matrix product operator* (MPO)



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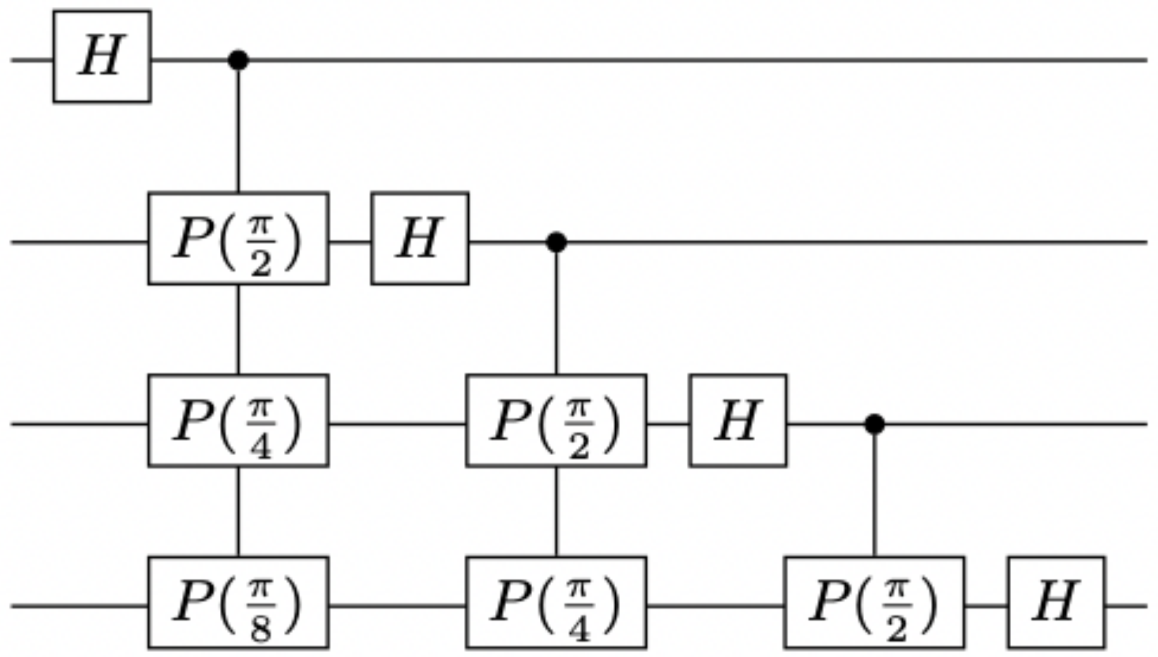
# Fourier transform

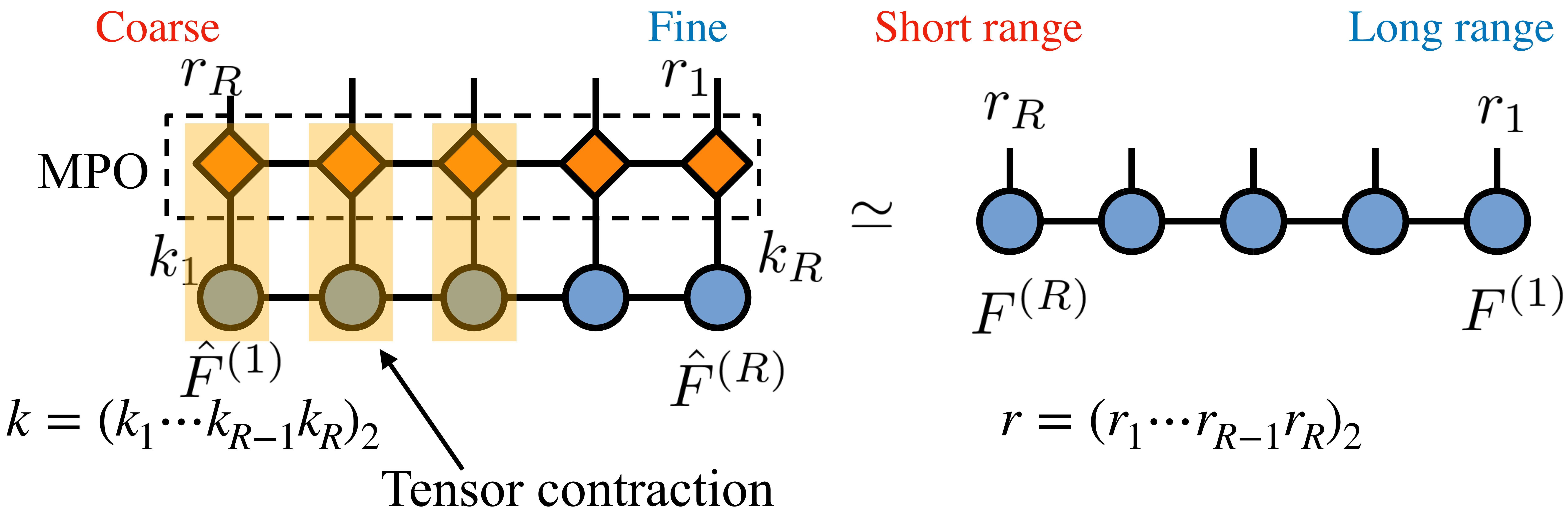



J. Chen *et al*., arXiv:2210.08468v1

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

Matrix product operator (MPO) for (quantum) 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



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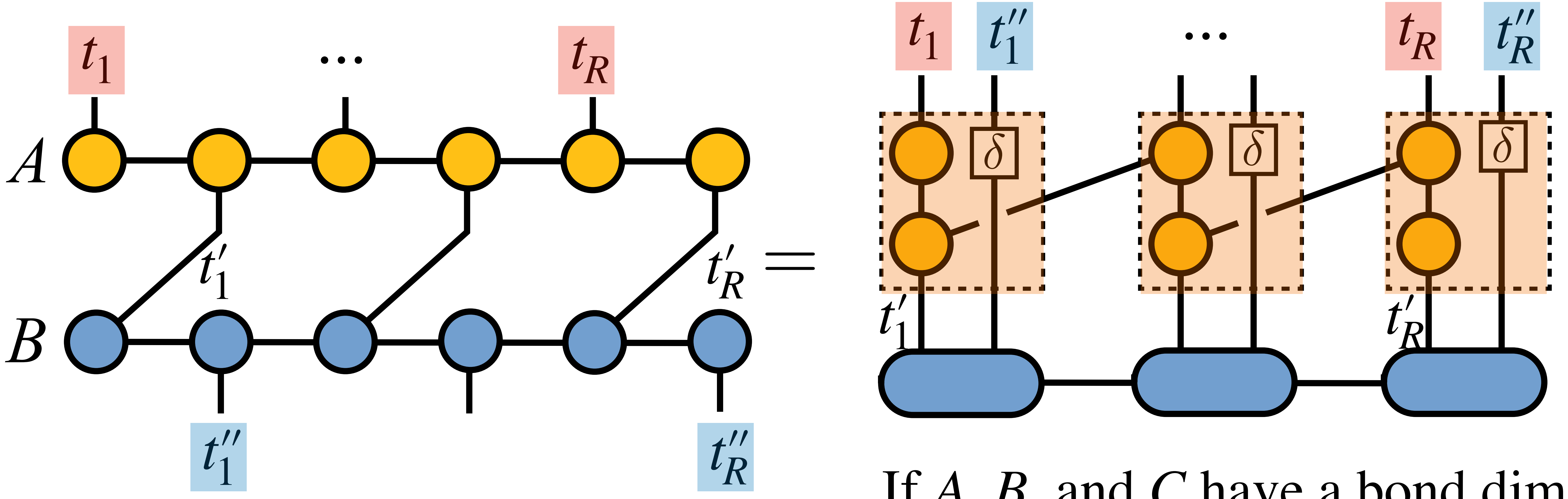
# Matrix multiplication

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

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

## Mapping to MPO-MPS multiplication




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

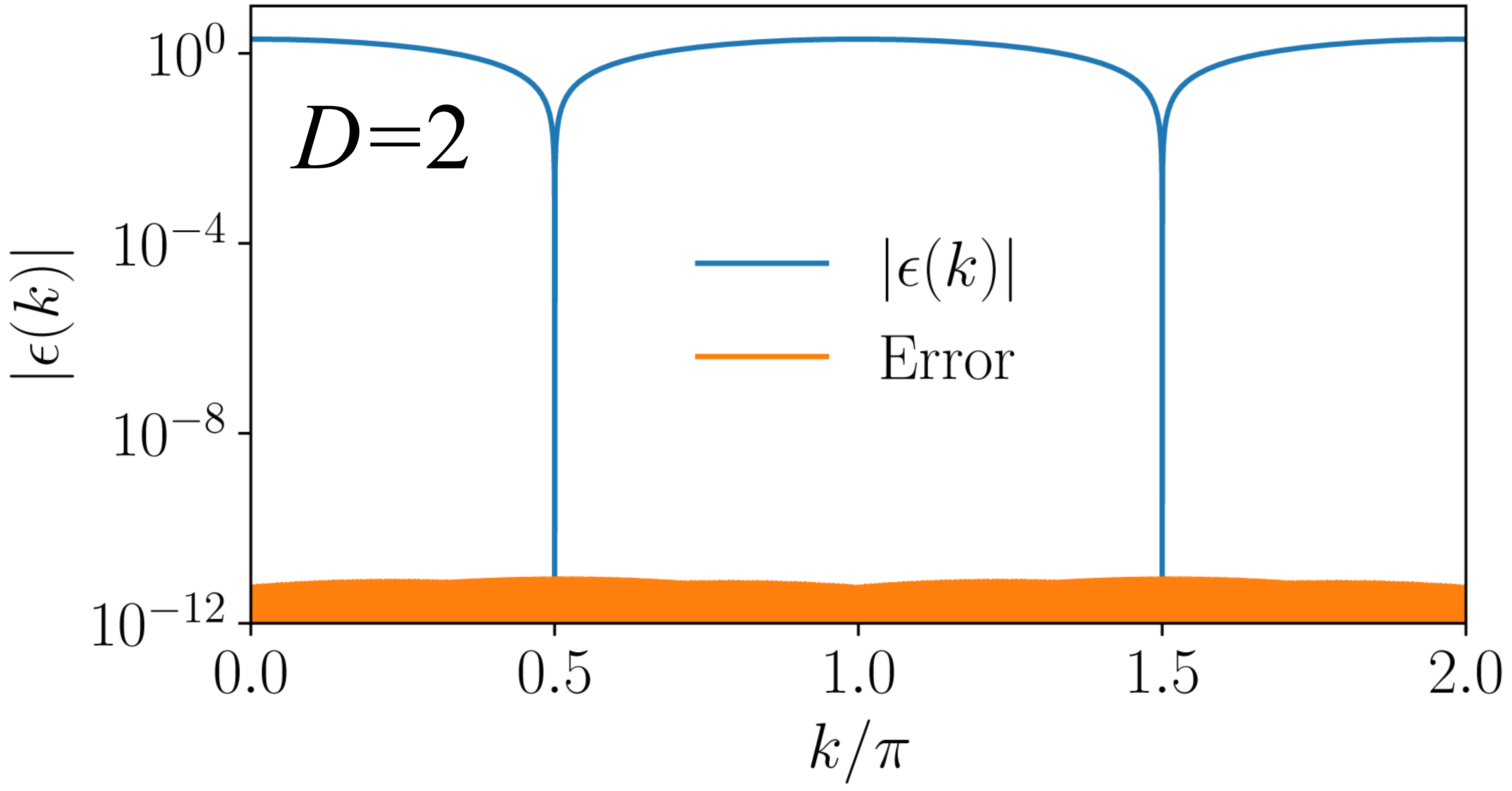


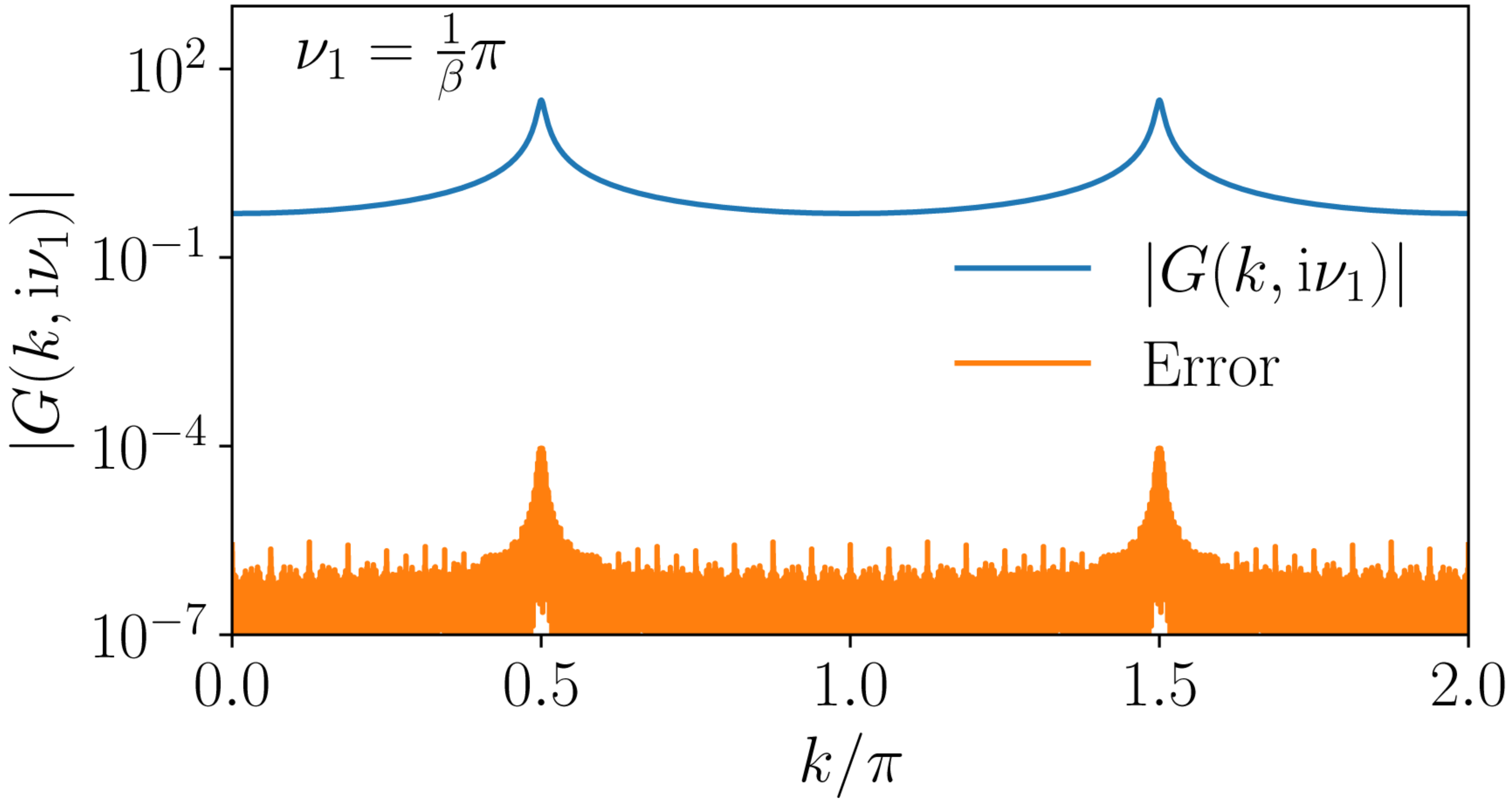
arXiv:2210.12984, arXiv:2303.11819

# Dyson equation

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

$$\epsilon(r) \xrightarrow{\text{QFT}} \epsilon(k) \xrightarrow{(\mathrm{i}\nu - \epsilon(k))G(k,\mathrm{i}\nu) = 1} G(k, \mathrm{i}\nu)$$



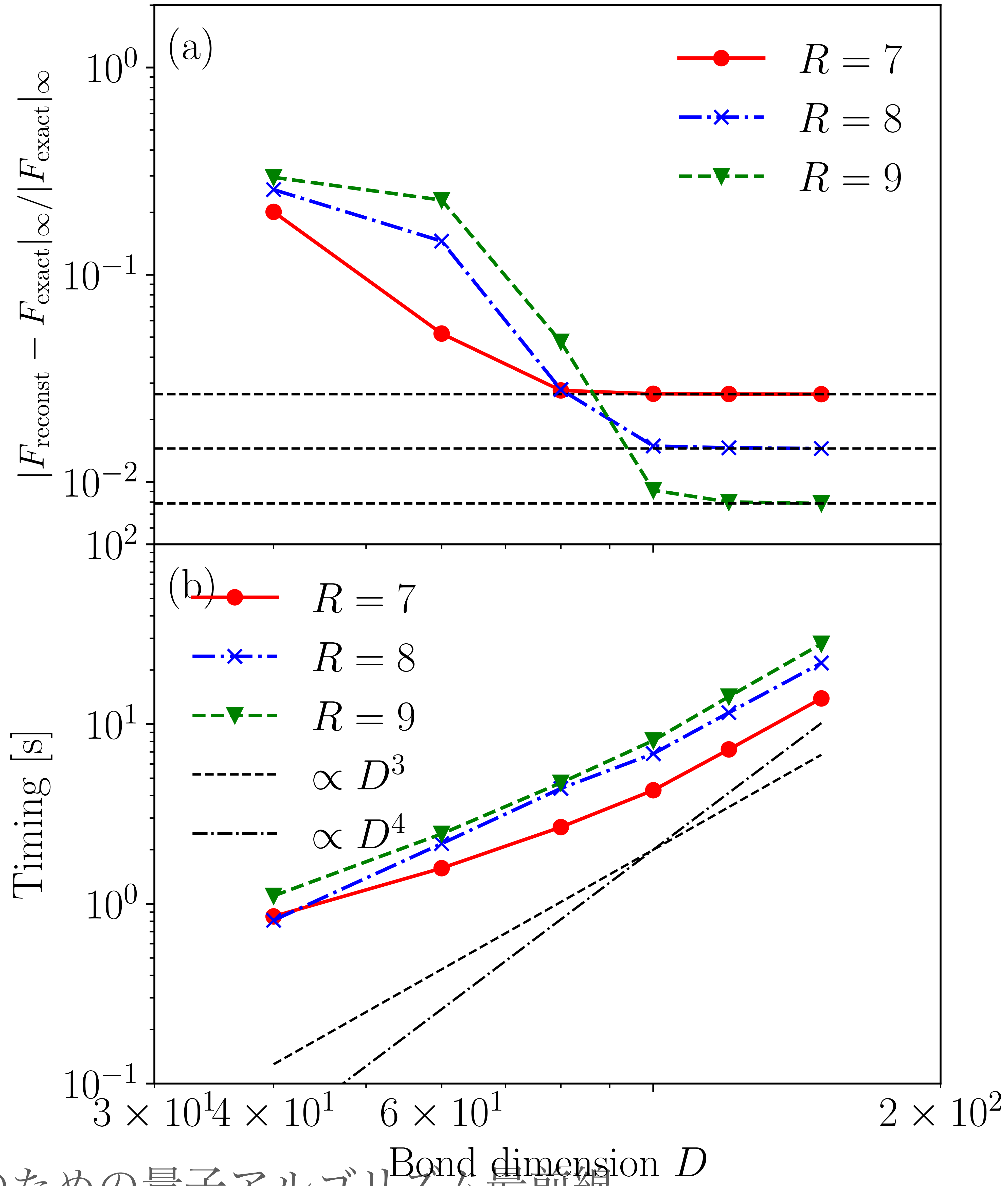

Exponential speed up



arXiv:2210.12984, arXiv:2303.11819

# Computation: Bethe-Salpeter equation

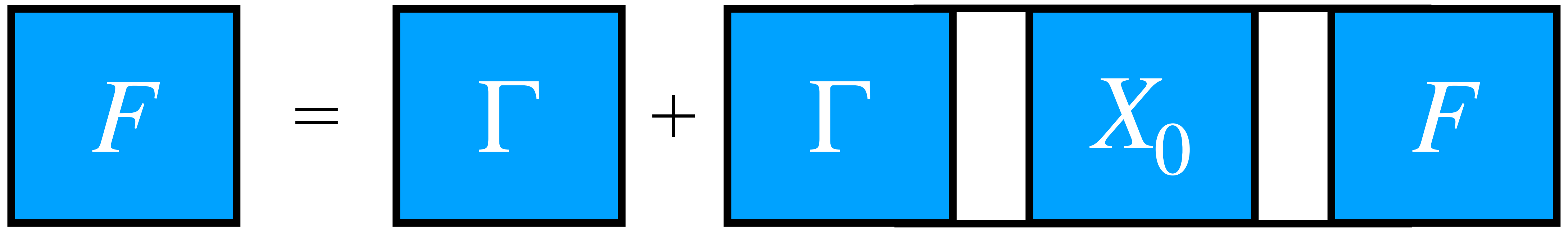
Particle-hole & density channel




Hubbard atom, $U$=3, $\beta$=1

One-shot evaluation of BSE

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




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

Exponential speed up



arXiv:2210.12984, arXiv:2303.11819

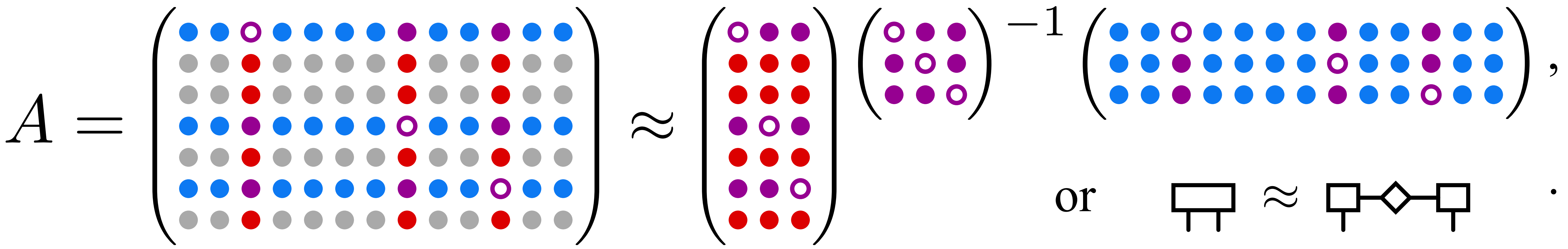
# Quantics tensor cross interpolation (QTCI)

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

## Constructing an MPS/TT from sampled values

### Matrix cross interpolation (MCI)

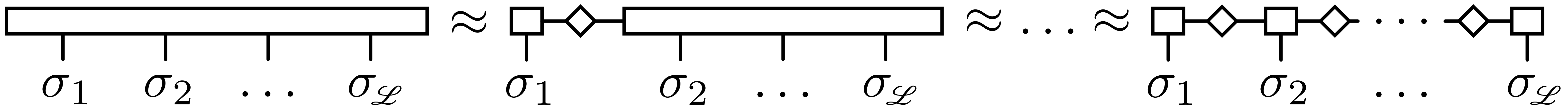
$$A \approx CP^{-1}R = \tilde{A}$$




### 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)

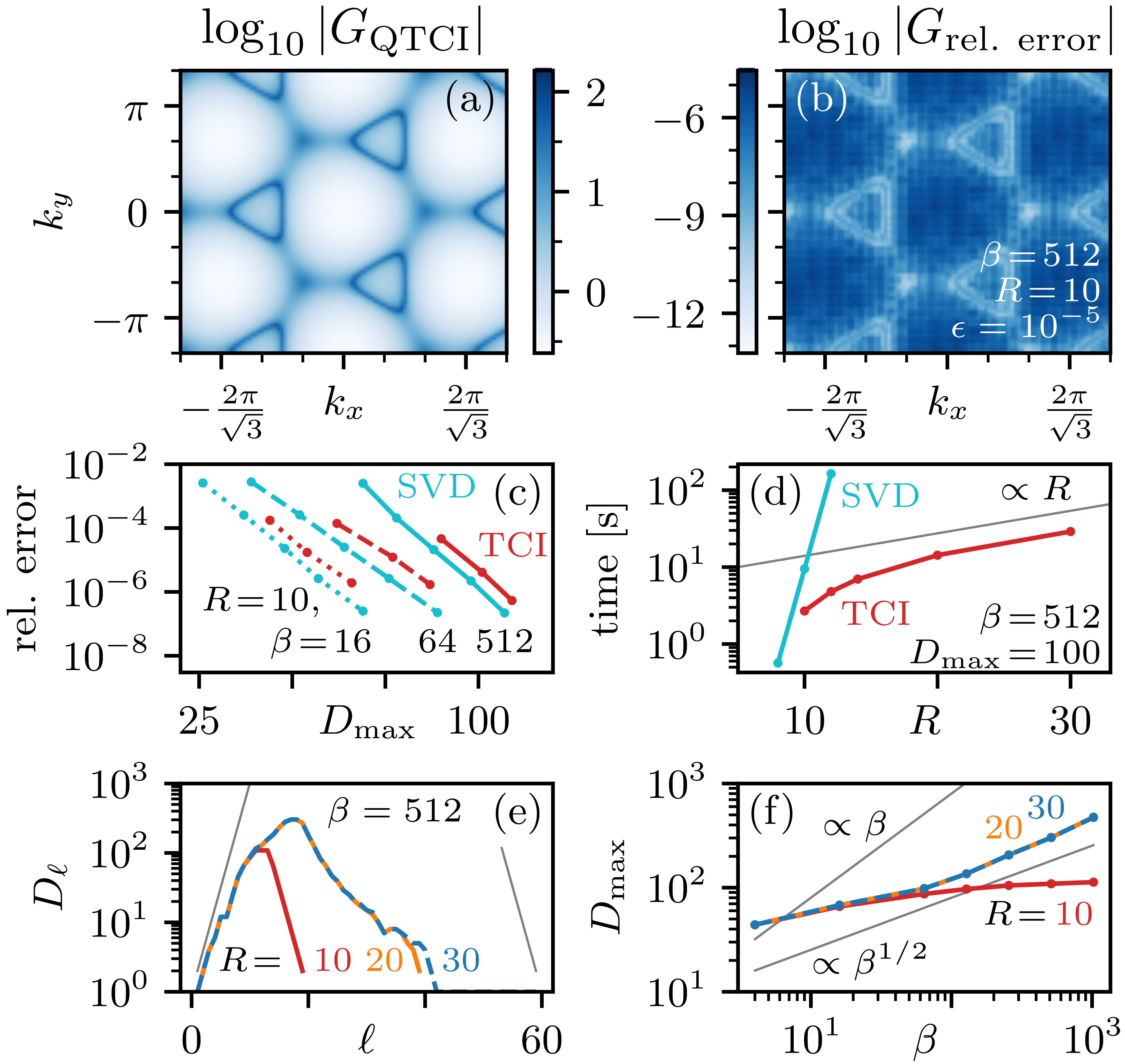



Stable and fast formula for constructing TT from sampled values of the function

Recent application to diagrammatic calculation: Y. N. Fernández *et al.*, PRX **12**, 041018 (2022)

# Quantics + TCI = QTCI

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




Non-interacting Green's function of the Haldane model

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

More results on Chern number in our preprint!



arXiv:2210.12984, arXiv:2303.11819

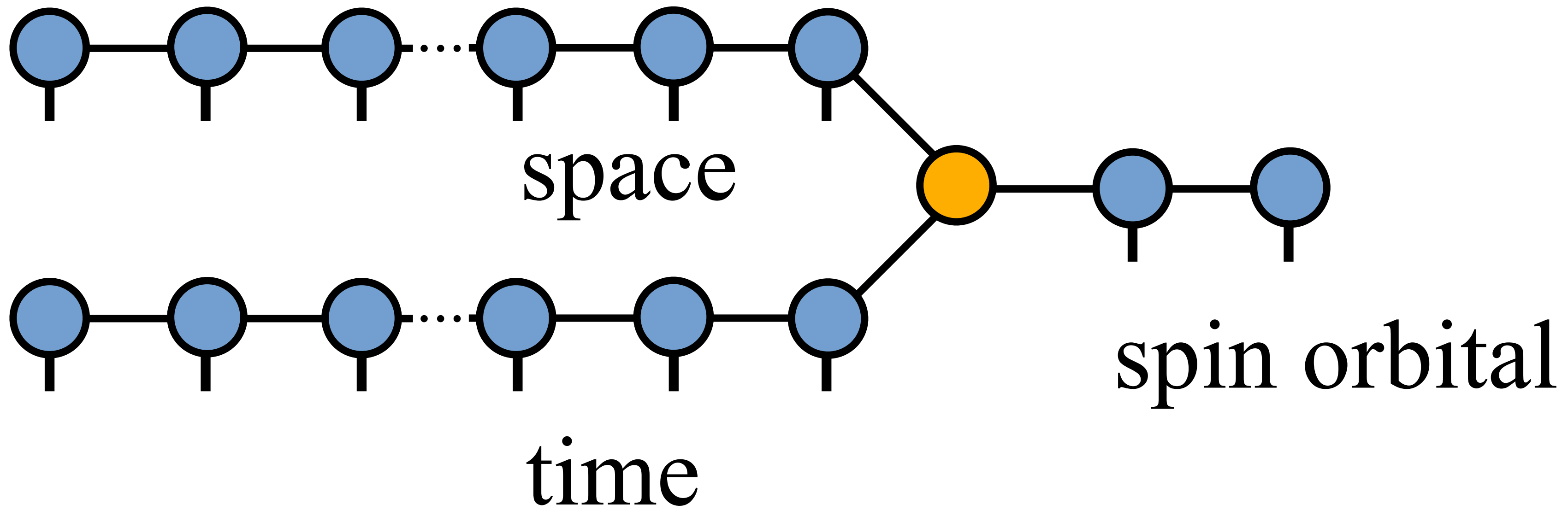
# Outlook

## From *ab-initio* to model/equilibrium to nonequilibrium calculations

- Non-local extension of DMFT
- *Ab-initio* fRG
- Vertex corrections: downfolding, Midal-Eliashberg equation, *GW* + BSE…
- Multi-orbital FLEX
- Nonequilibrium simulations…

## Remaining issues

Object depending space & time & spin-orbital




Efficient parallelization of MPO-MPS multiplication

Can we implement QTT on a real quantum computer?



arXiv:2210.12984, arXiv:2303.11819

# Collaborators

**Saitama Univ.**
Rihito Sakurai

**TU Wien**
Markus Wallerberger
Anna Kauch

**Kyoto Univ.**
Kosuke Nogaki

**Fribourg Univ.**
Philipp Werner

**Riken**
Yuta Murakami

**LMU Munich**
M. K. Ritter
J. von Delft

**CEA Grenoble**
Y. N. Fernández
X. Waintal

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



arXiv:2210.12984, arXiv:2303.11819

# Summary

Multiscale space-time ansatz based on quanticsd tensor trains

- Exponentially wide range of length scales
  from equilibrium to non-equilibrium systems
- Systematic error control by bond dimension
- Computation
  Fourier transform, convolution, QTCI, *etc*.

HS, M. Wallerberger, Y. Murakami, K. Nogaki, R. Sakurai, P. Werner, A. Kauch, arXiv:2210.12984v2 (to appear in PRX)
M. K. Ritter, Y. N. Fernández, M. Wallerberger, J. von Delft, HS, X. Waintal, arXiv:2303.11819

2023〜2025年度: 学術変革領域研究B「量子古典融合アルゴリズムが拓く計算物質科学 」品岡*、大久保、水上 (+分担)
2024年度〜 (基本7年)　JST創発 「2粒子レベルの量子埋め込み理論に基づく新規第一原理計算手法の開発と実証」