Quantics Tensor Trains meet quantum field theories

Exploiting *scale separation*

Hiroshi SHINAOKA

Saitama University

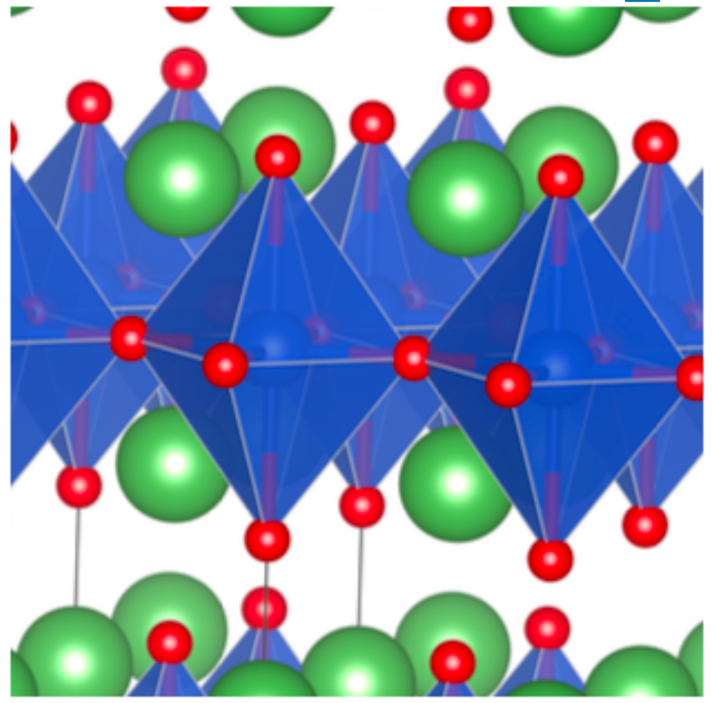
Baesd on PRX **13**, 021015 (2023), PRL **132**, 056501 (2024) and many others!

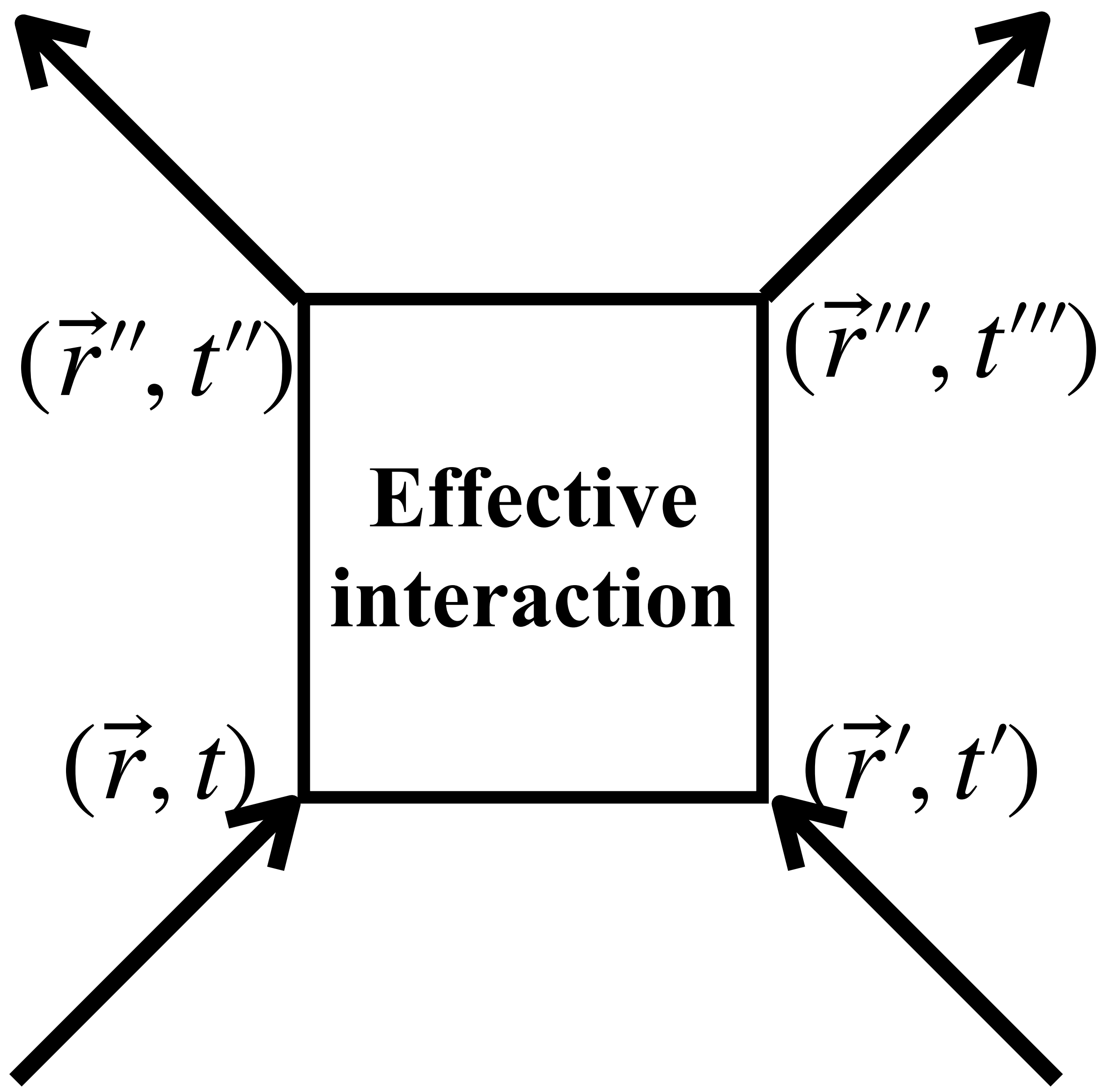
Quantum field theories and dimensionality reduction

Novel diagrammatic theories

Migal-Eliashberg theory, *GW*, dynamical mean-field theory, functional RG, …

Novel correlated physics





Numerical obstacles

- Coexisting scales (e.g., bandwidth vs Kondo temperature)
- Multi space-time coordinates, spin, orbitals
- Convolution, Fourier transform…

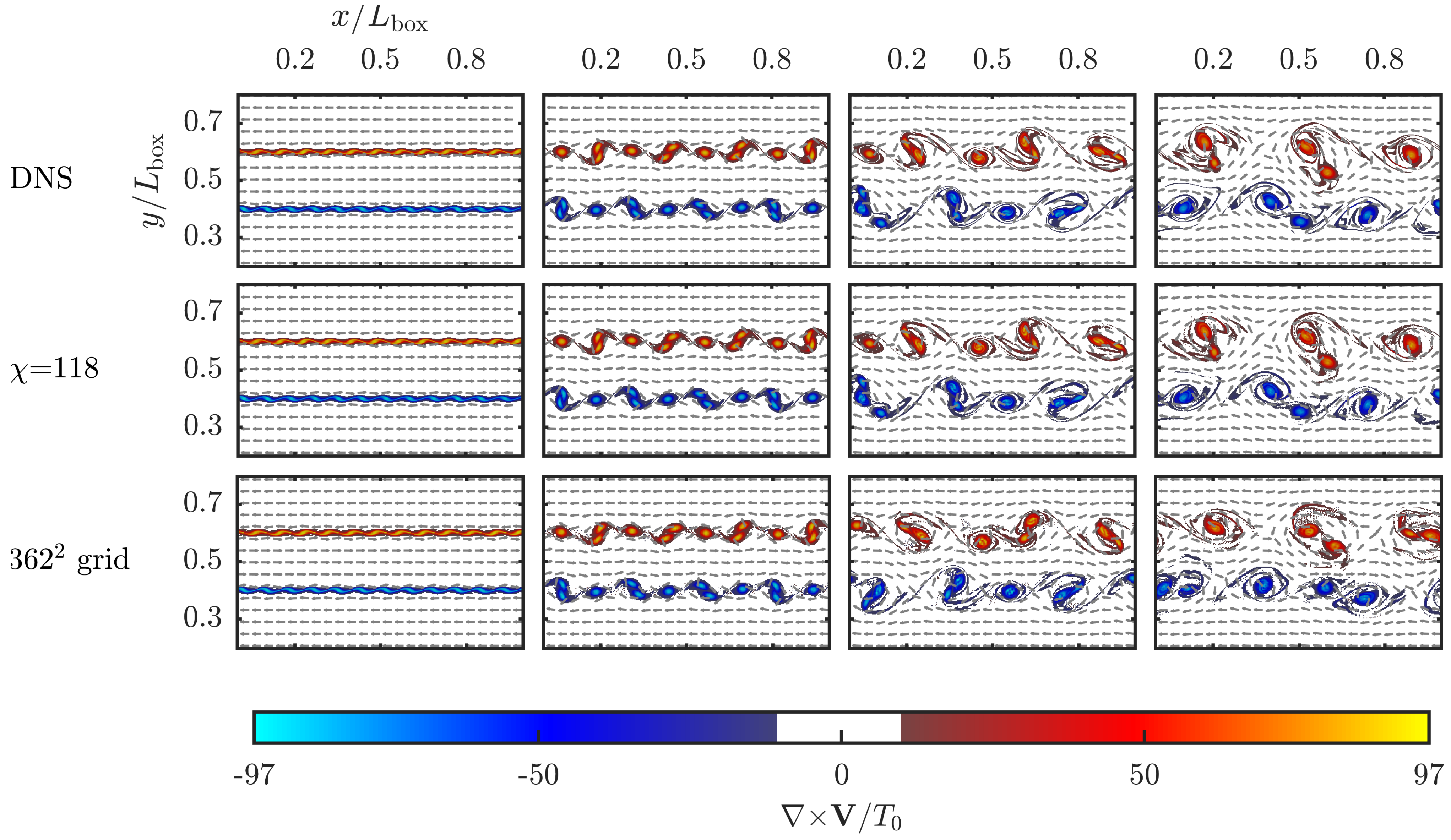
Our idea: Use scale separation!

Scale separation

A new structure we can exploit for efficient computation through *quantics tensor trains (QTT)*

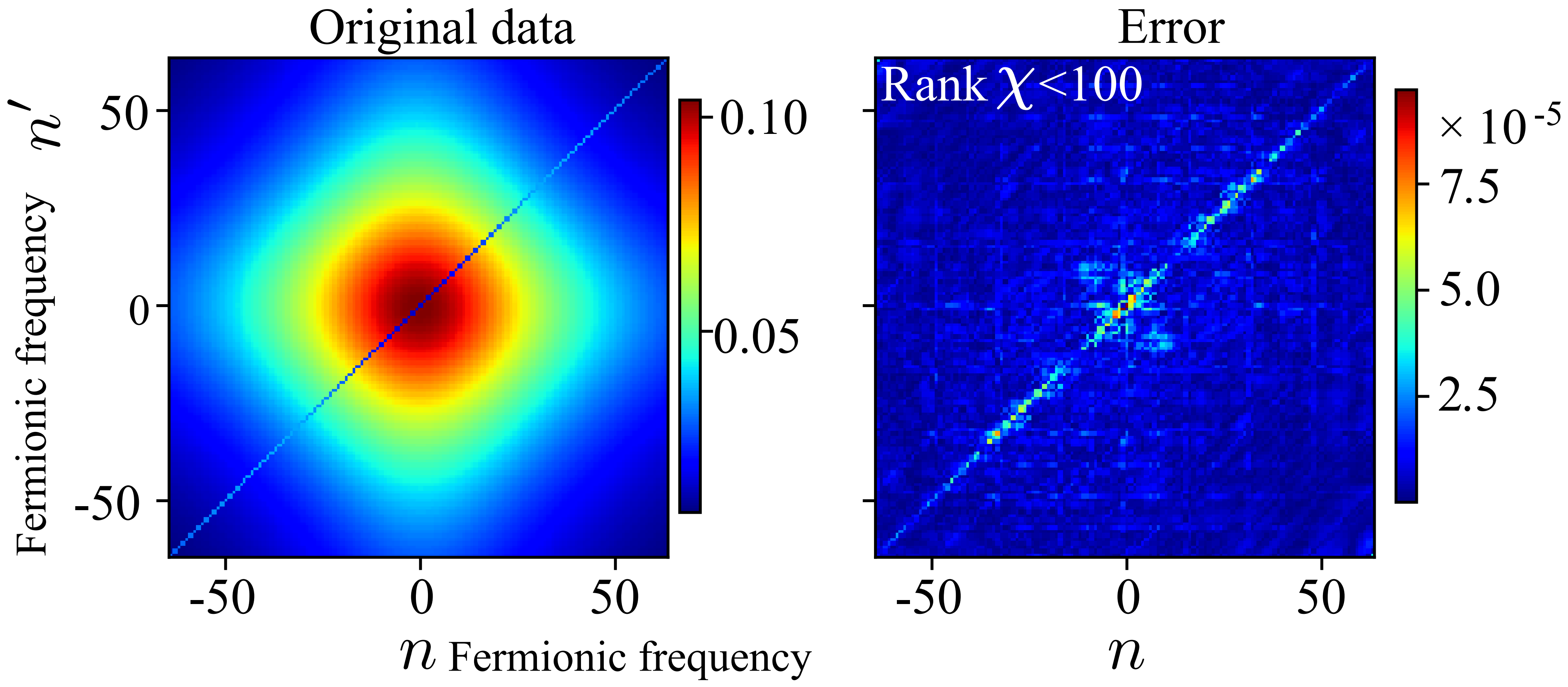
Solving Navier-Stokes equations for turbulent flows

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



Quantum field theories

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



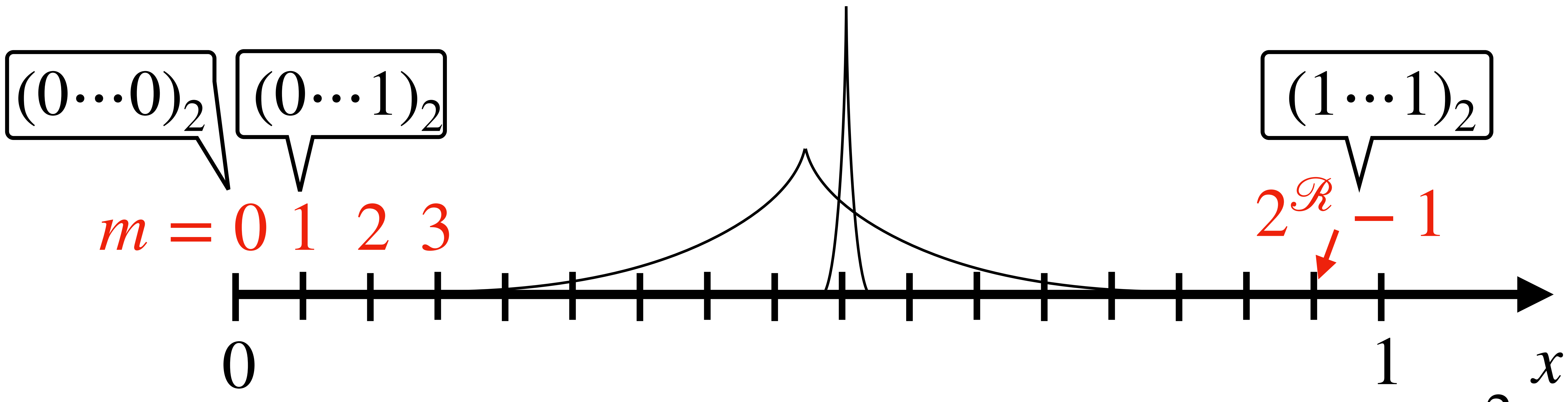
Vlasov-Poisson equations for collisionless plasmas

E. Ye and N. F. G. Loureiro, PRE **106**, 035208 (2022)

and more and more!

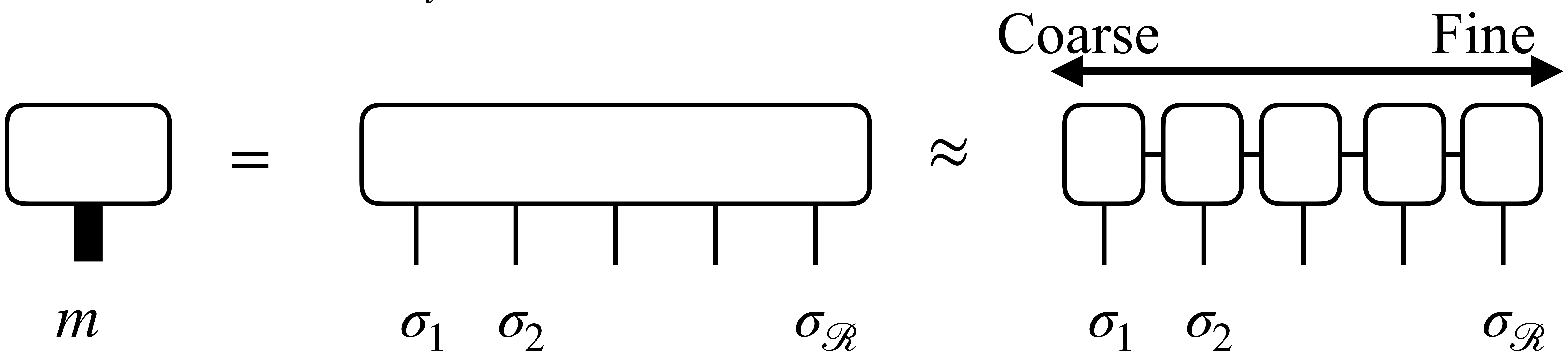
Quantics Tensor Train (QTT)

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



Binary coding $m = (\sigma_1\sigma_2\cdots\sigma_{\mathscr{R}})_2$ $\qquad x_m = \sigma_1/2 + \sigma_2/2^2 + \cdots + \sigma_{\mathscr{R}}/2^{\mathscr{R}}$

$\sigma_l \in \{0,1\}$



Exponentially fine resolution, multivariate variables, computable!

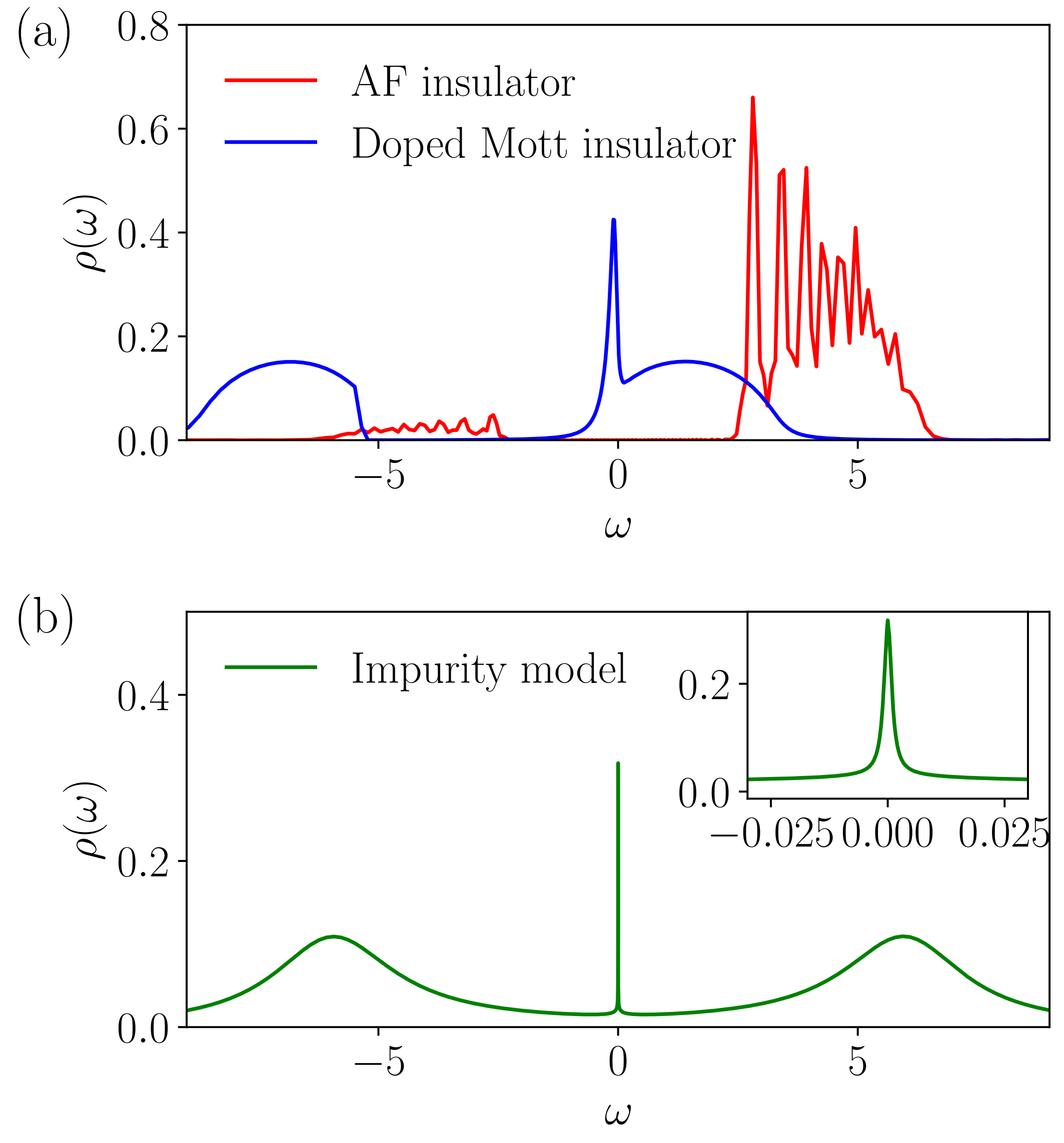
See later slides

Scale separation in correlation functions of quantum systems

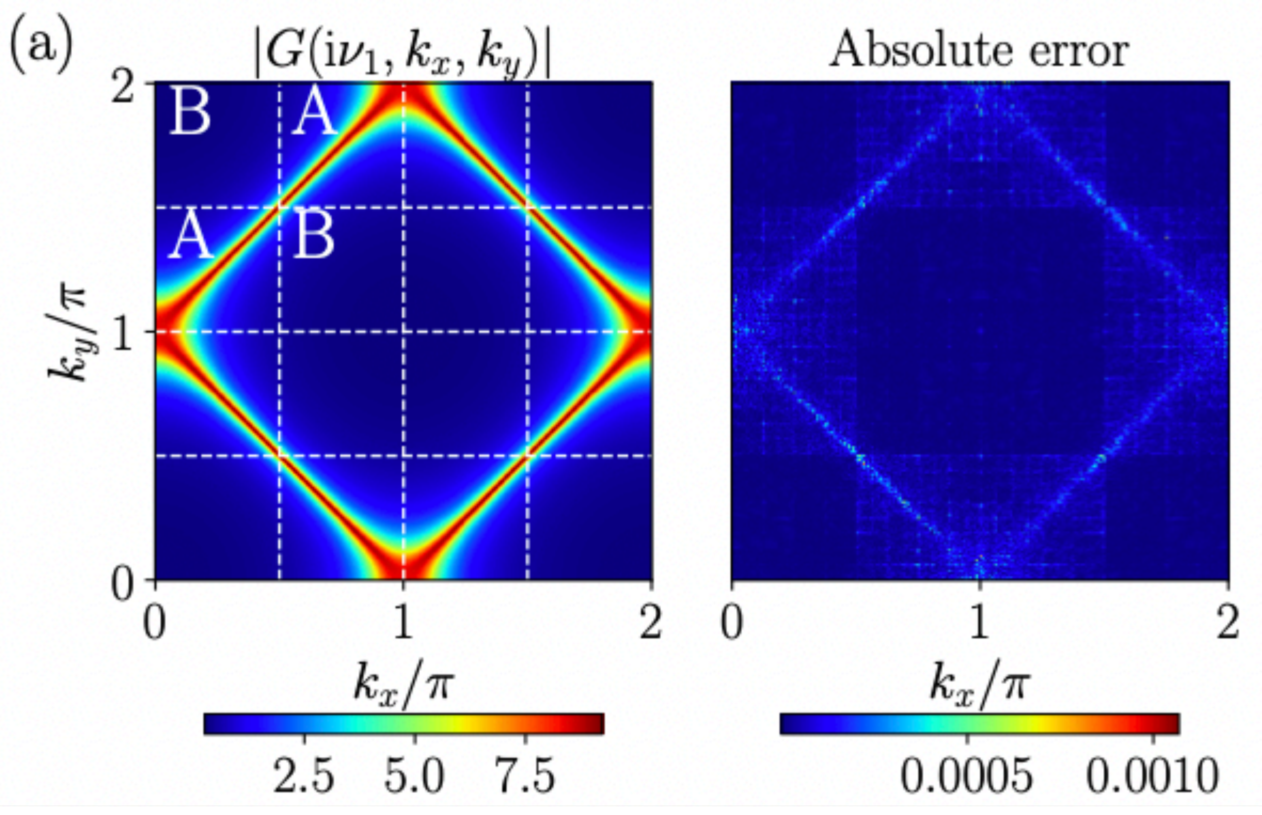
Space-time dependence of correlation functions are compressible!

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

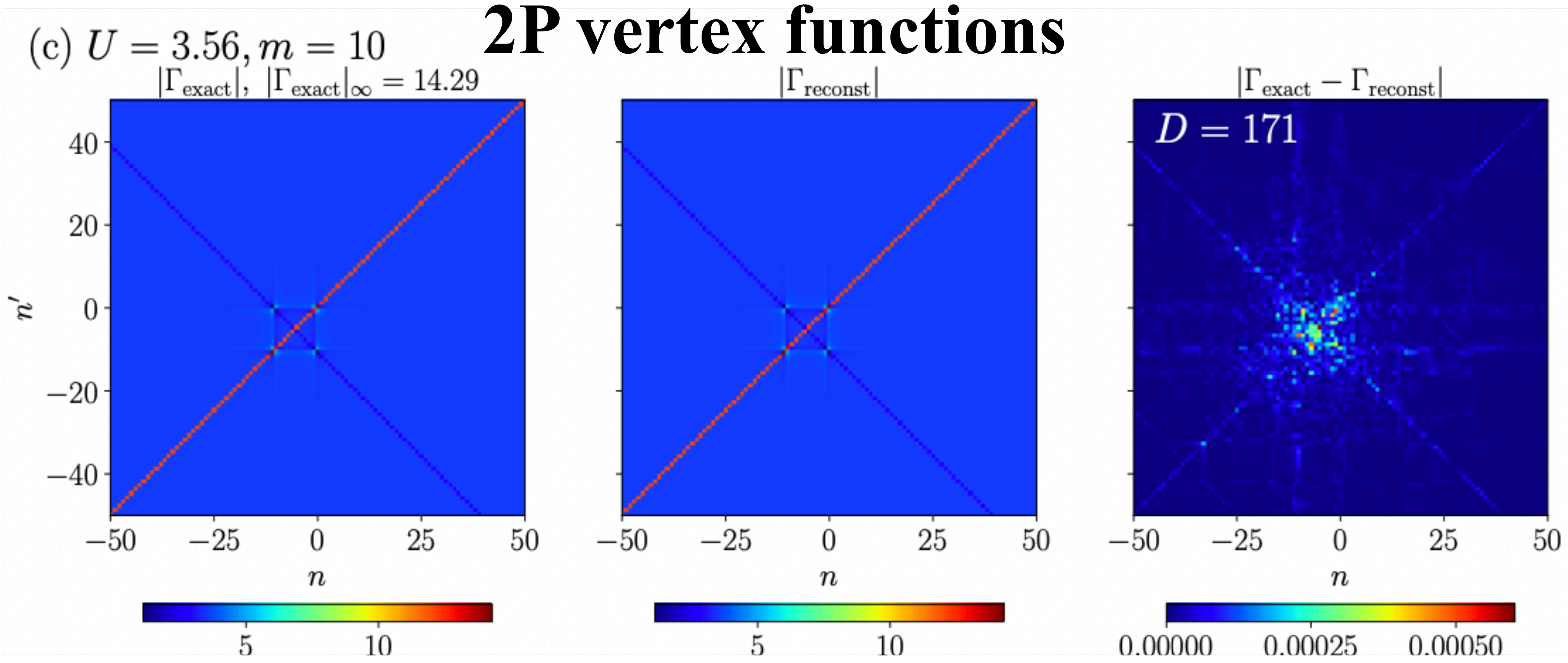
Spectral function



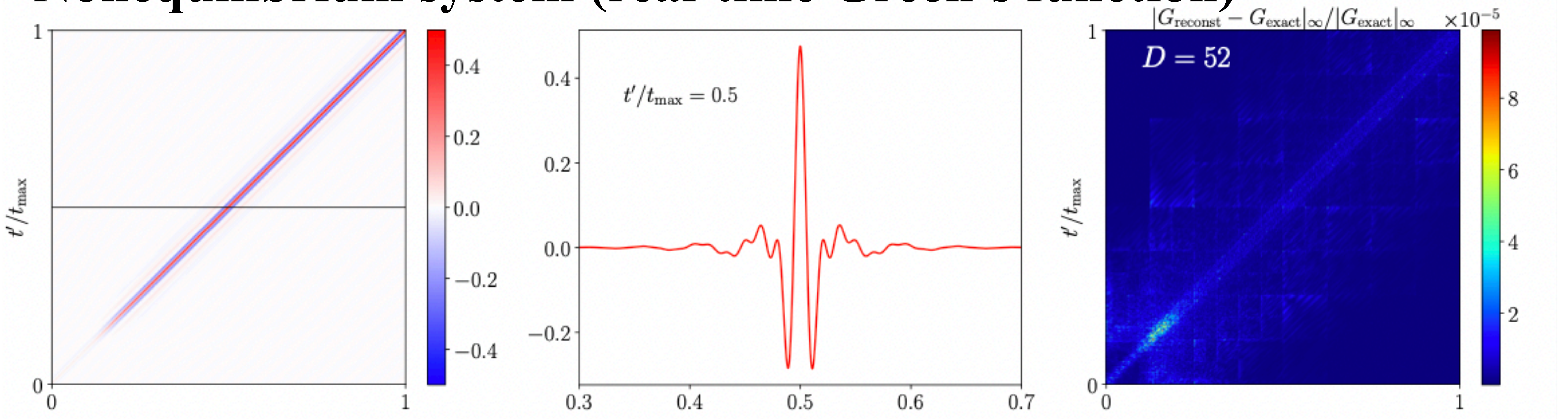
1P momentum space



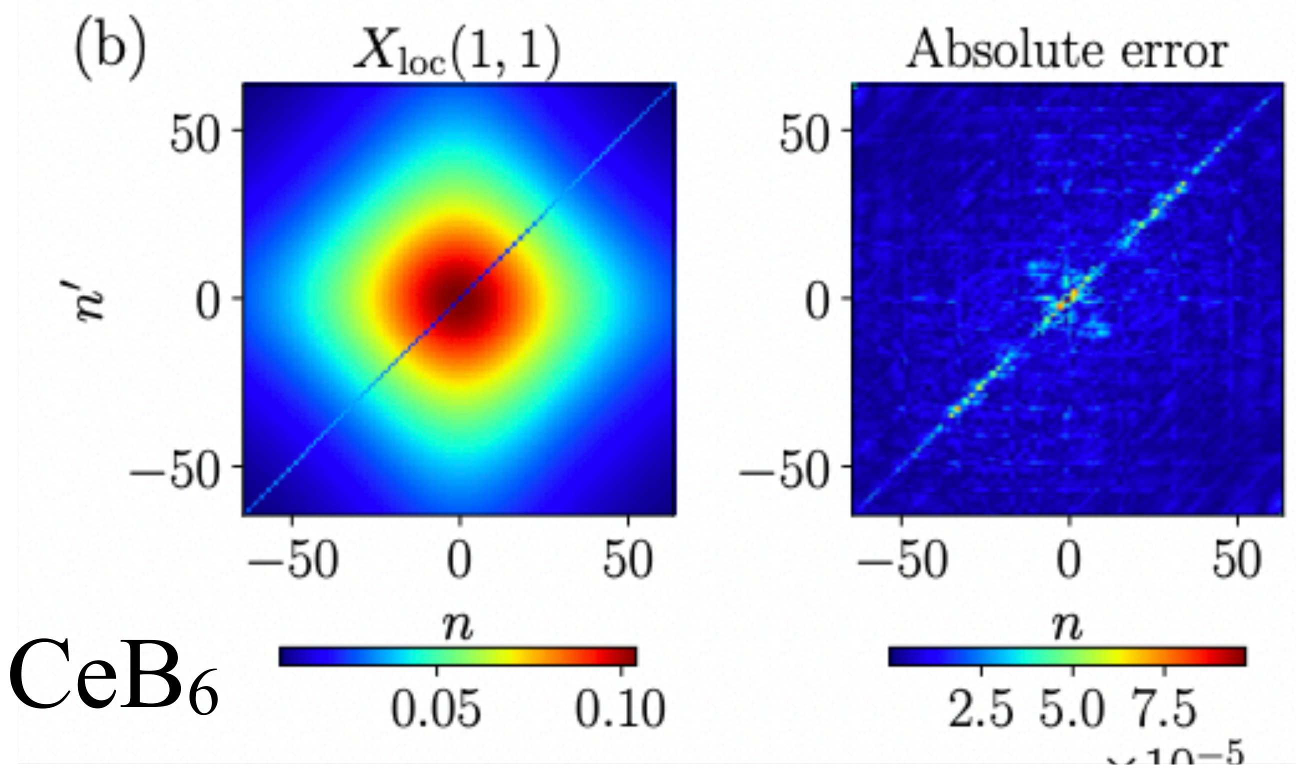
2P vertex functions



Nonequilibrium system (real-time Green's function)



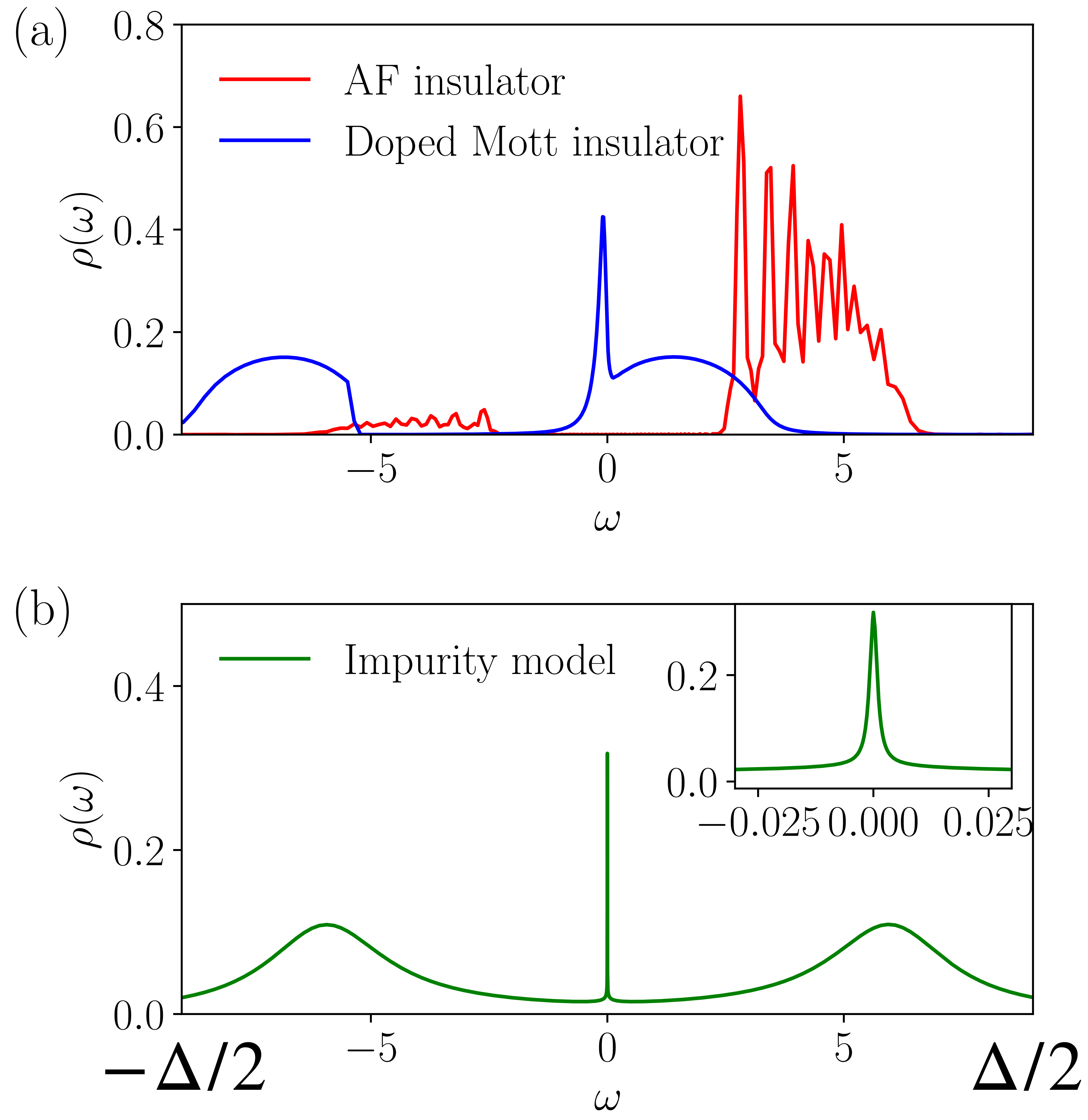
Multipolar susceptibility

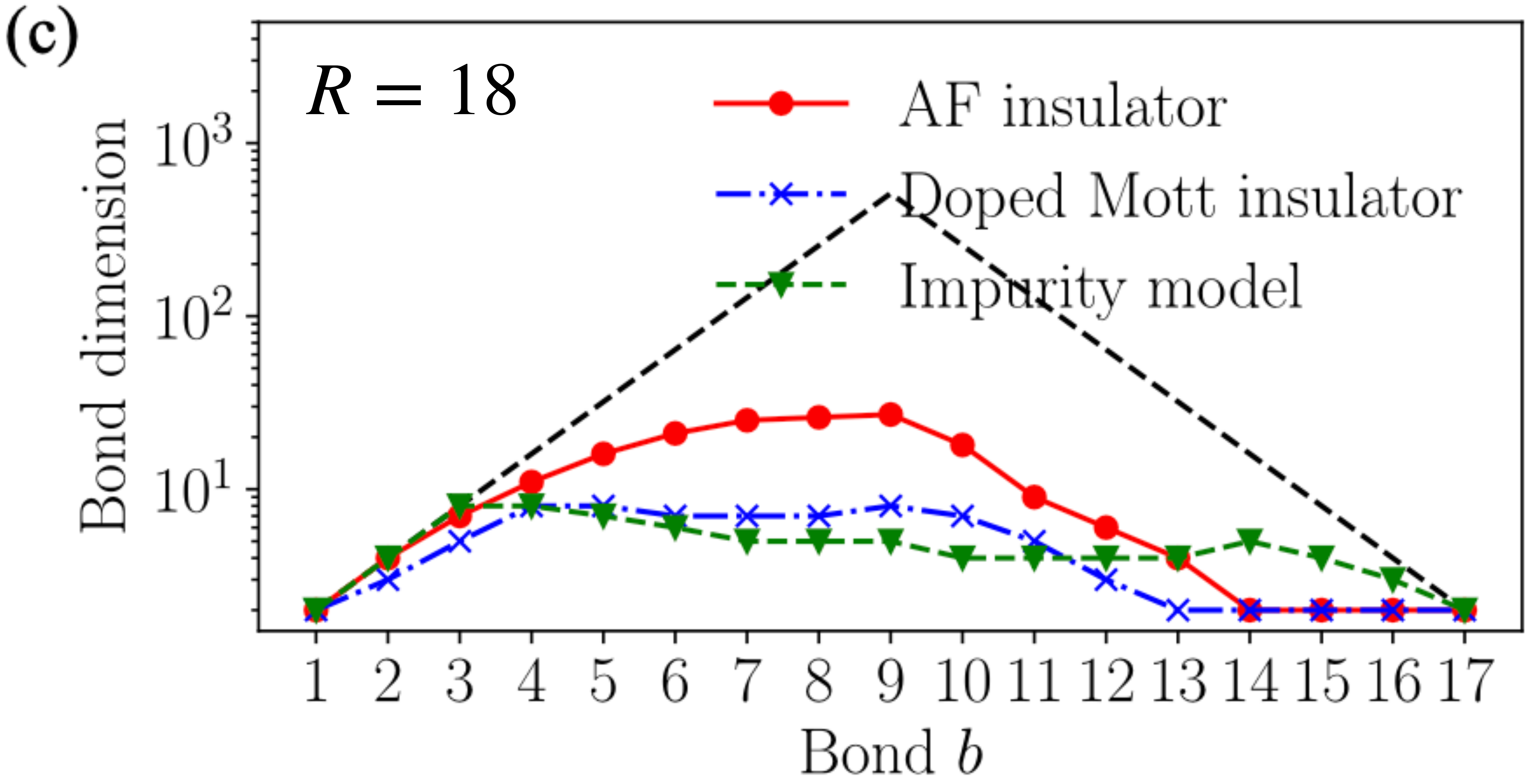


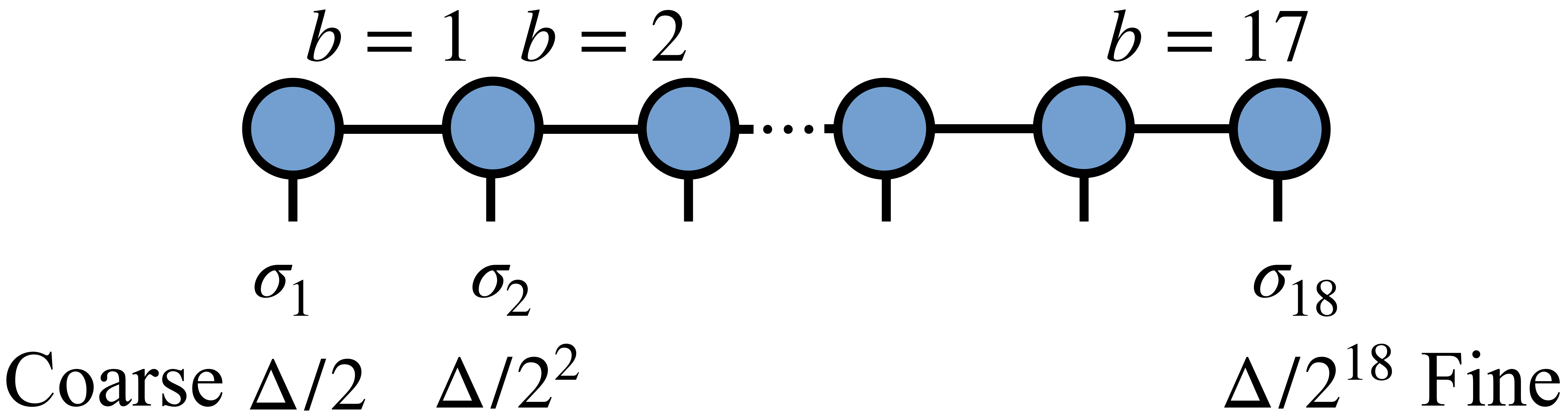
CeB_6

Quantum impurity model

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

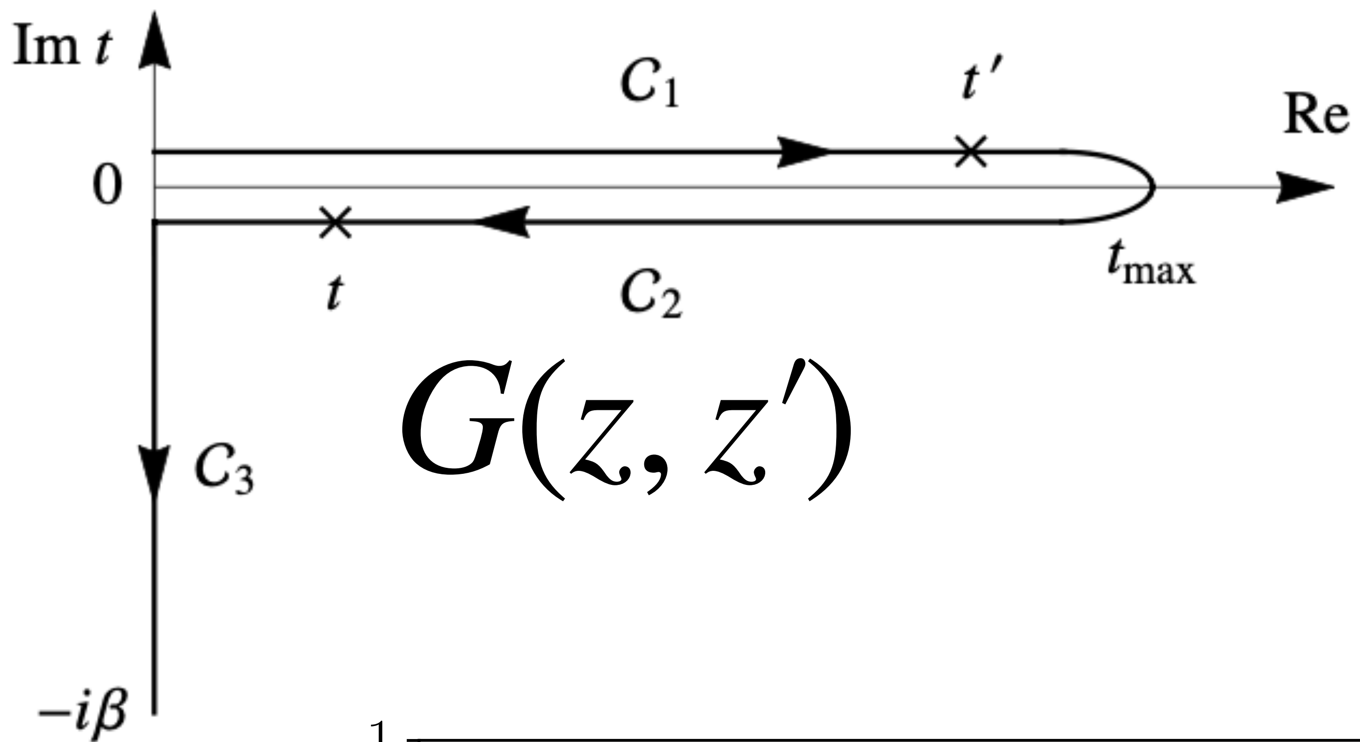


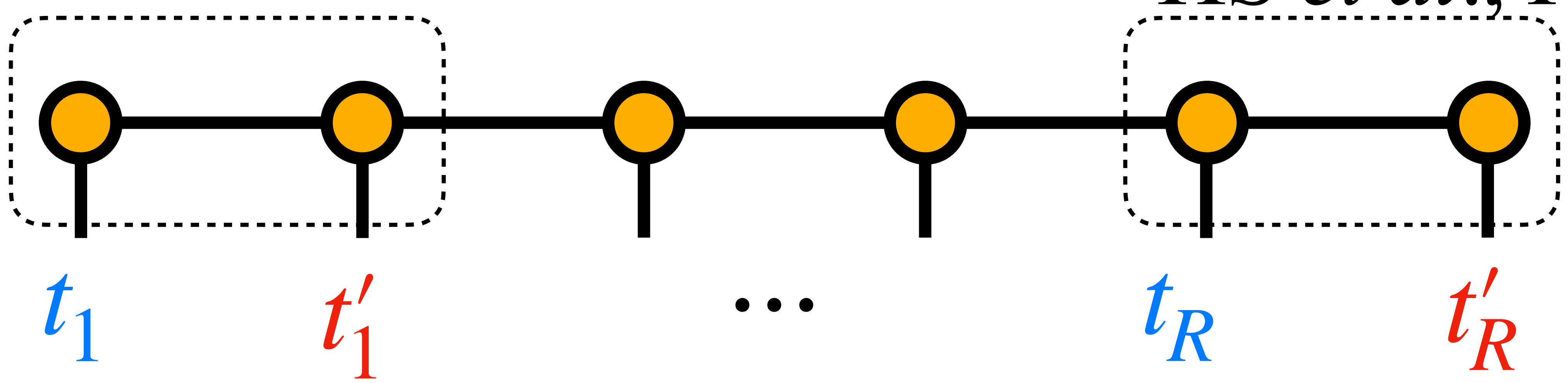




Keldysh Green's function: Non-equilibrium case

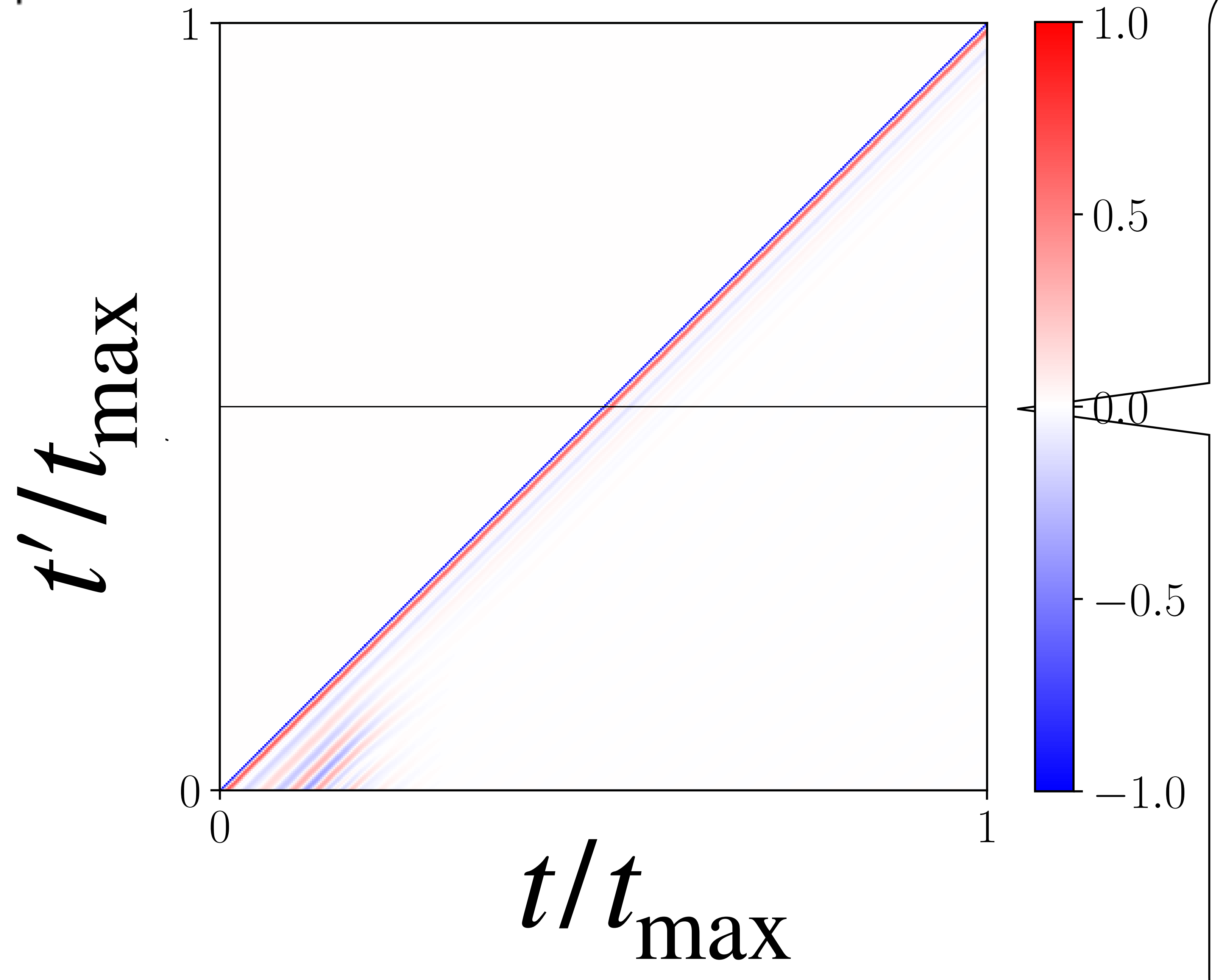
HS *et al.*, PRX **13**, 021015 (2023



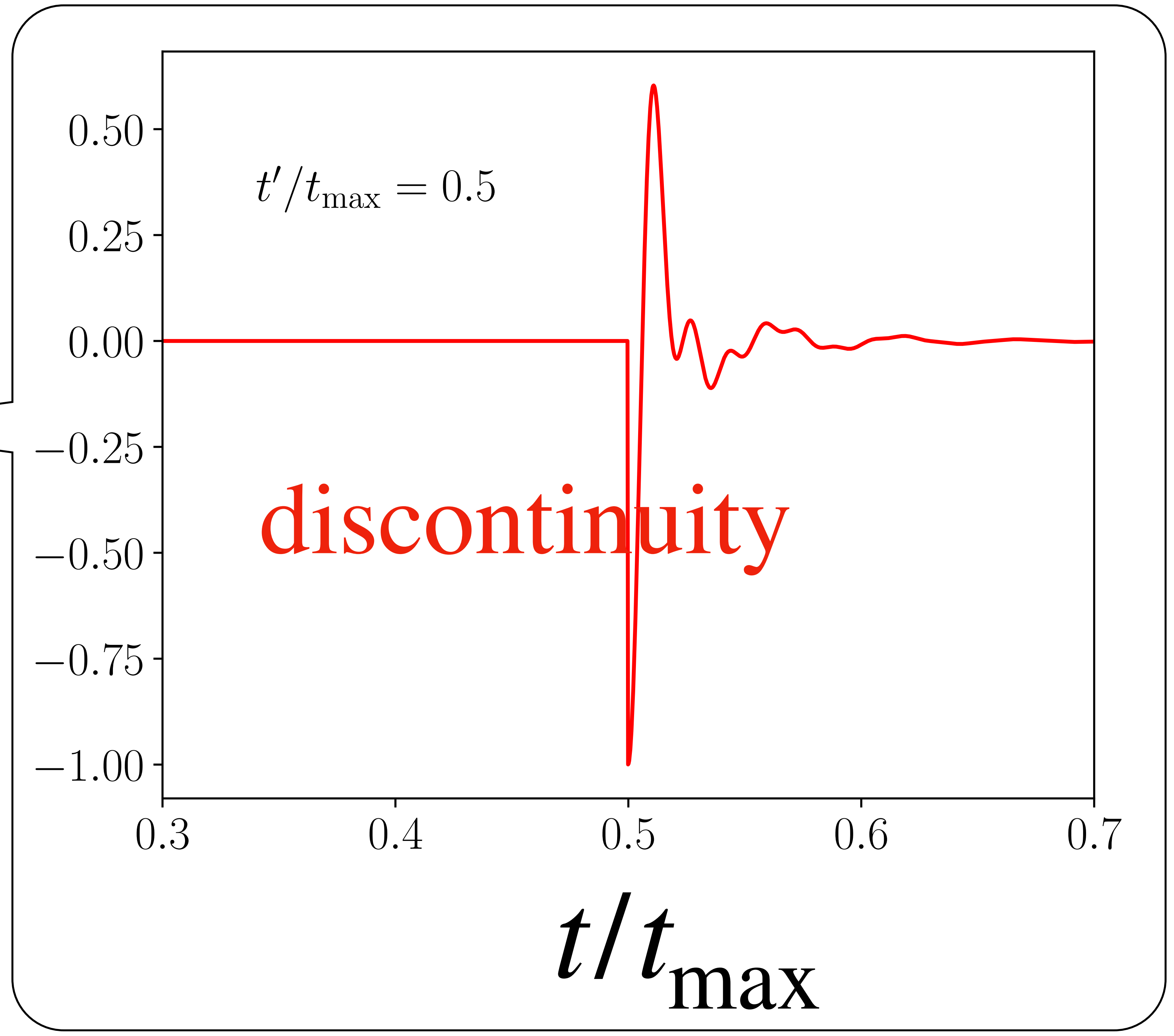


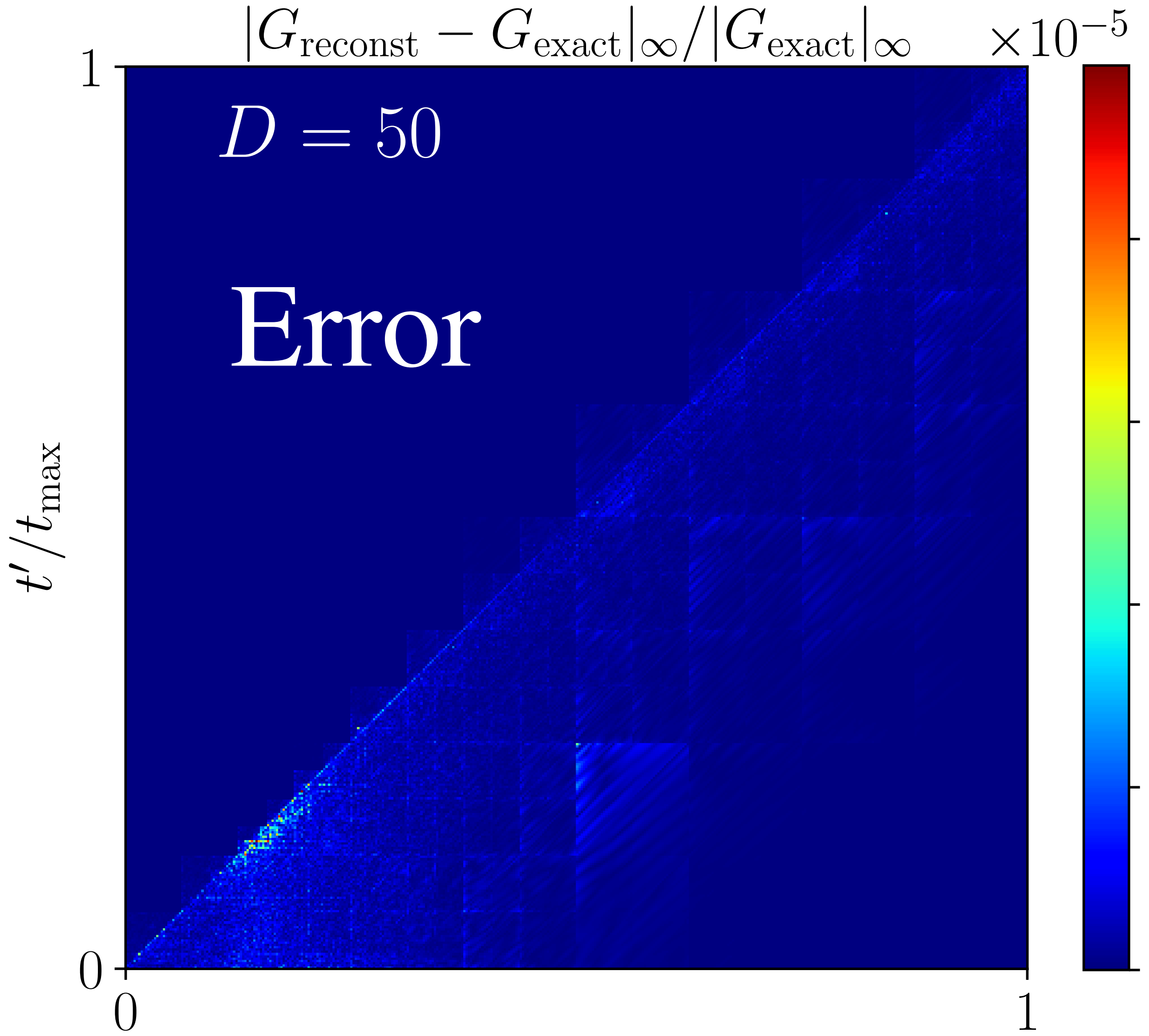
Interleaved representation

$$t/t_{\mathrm{max}} = (0.t_1 \cdots t_R)_2,\ t'/t_{\mathrm{max}} = (0.t'_1 \cdots t'_R)_2$$



slow to long dynamics





compression ratio ~ 1000

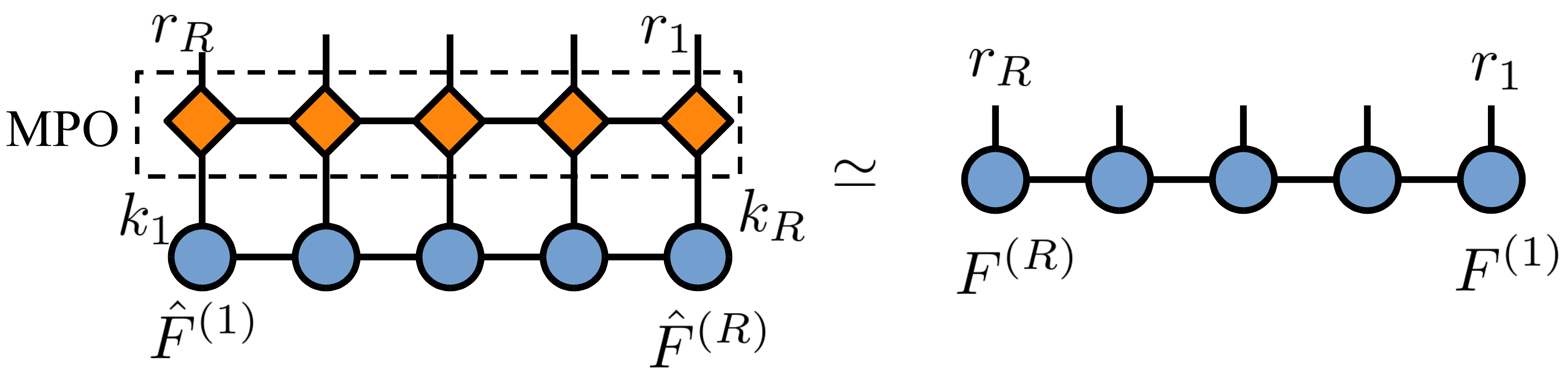
Low-T AF Mott phase excited by a short electric field pulse, Bethe lattice, $T = 0.05$

Computation in QTT with exponentially small discretization error

Fourier transform

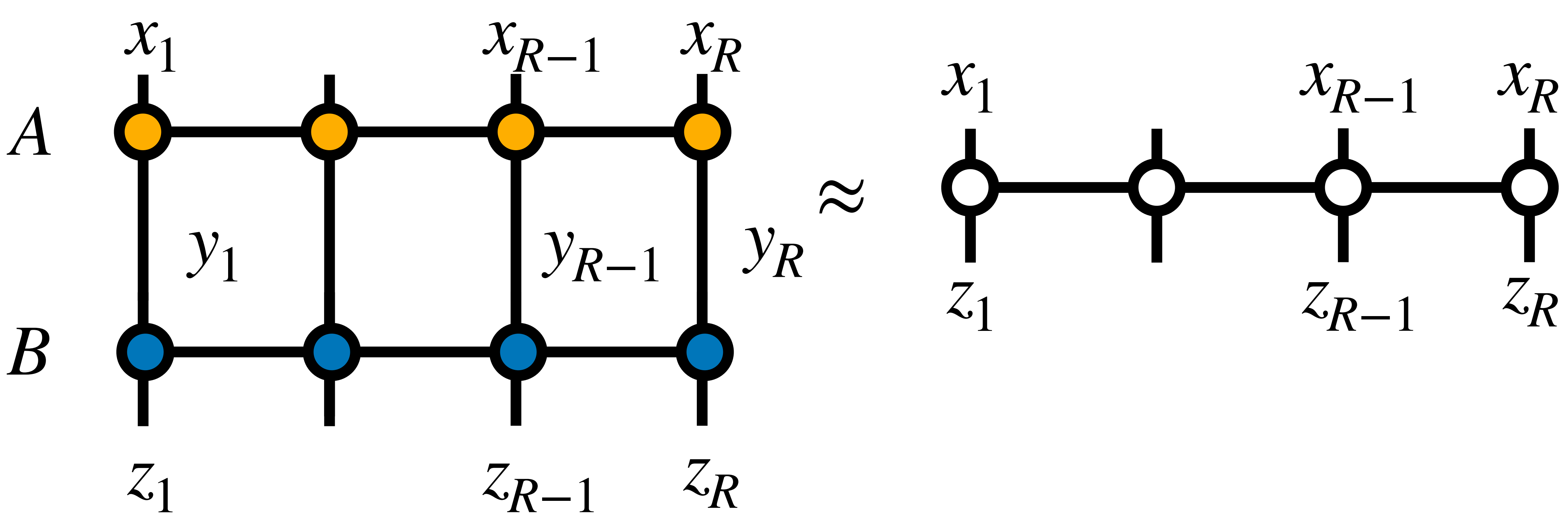
K. J. Woolfe *et al.*, Quantum Inf. Comput. **17**, 1 (2017) , **HS** *et al.*, PRX **13**, 021015 (2023), J. Chen, E.M. Stoudenmire, S. R. White, PRX Quantum **4**, 040318 (2023)

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



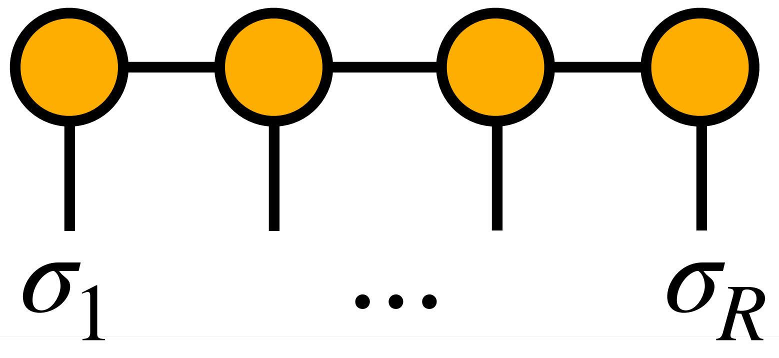
Convolution

$$\int dy\ A(x,y)\ B(y,z) \qquad C(x,z)$$



Integration

$$\int dx\ f(x) \simeq 2^{-R} \sum_{\sigma_1, \cdots \sigma_R}$$

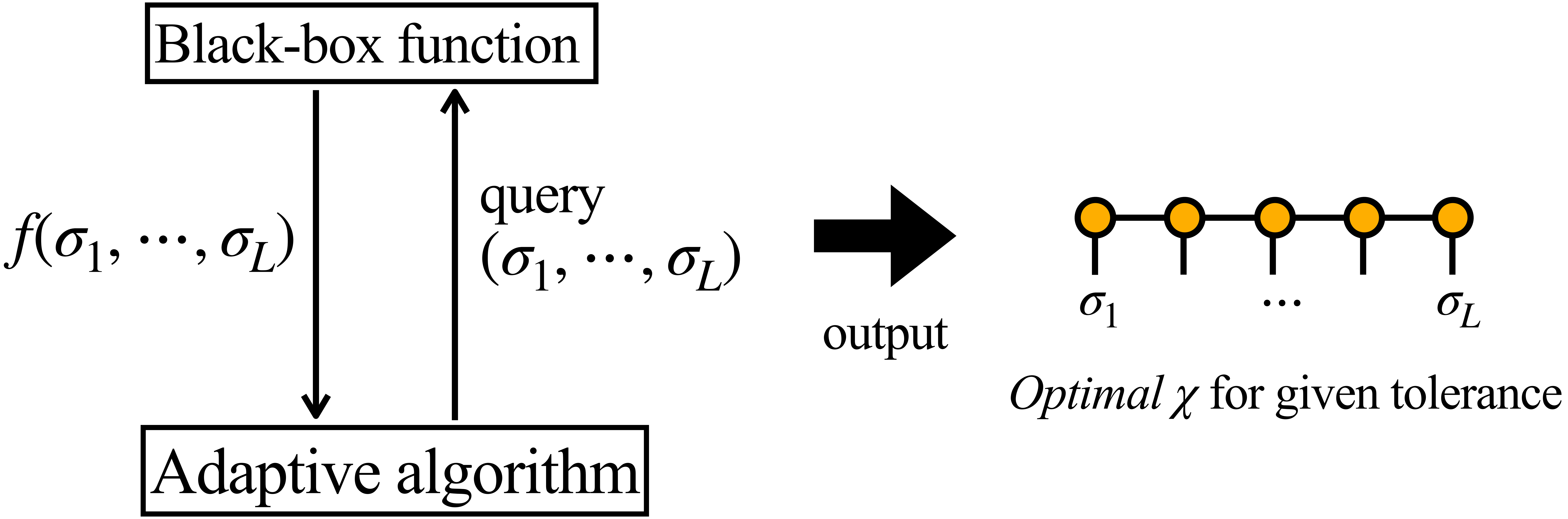


- Solving linear equations and differential equations are straightforward.
- Combination with *Tensor Cross Interpolation (TCI)* is advantageous.

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)
Y. Núñez Fernández *et al.*, PRX **12**, 041018 (2022)
Y. Núñez Fernández, M. K. Ritter, M. Jeannin, J.-W. Li, T. Kloss, T. Louvet, S. Terasaki, O. Parcollet, J. von Delft, **HS**, X. Waintal, SciPost Phys. **18**, 104 (2025).

Input:
- $f(\sigma_1, \cdots, \sigma_L)$
- initial *pivots*



- Read $O(\chi^2 L)$ elements; the function can be computed on the fly.
- Fast learning without gradient descent

Quantics + TCI = QTCI

M. K. Ritter, …, **HS**, and X. Waintal, PRL **132**, 056501 (2024)

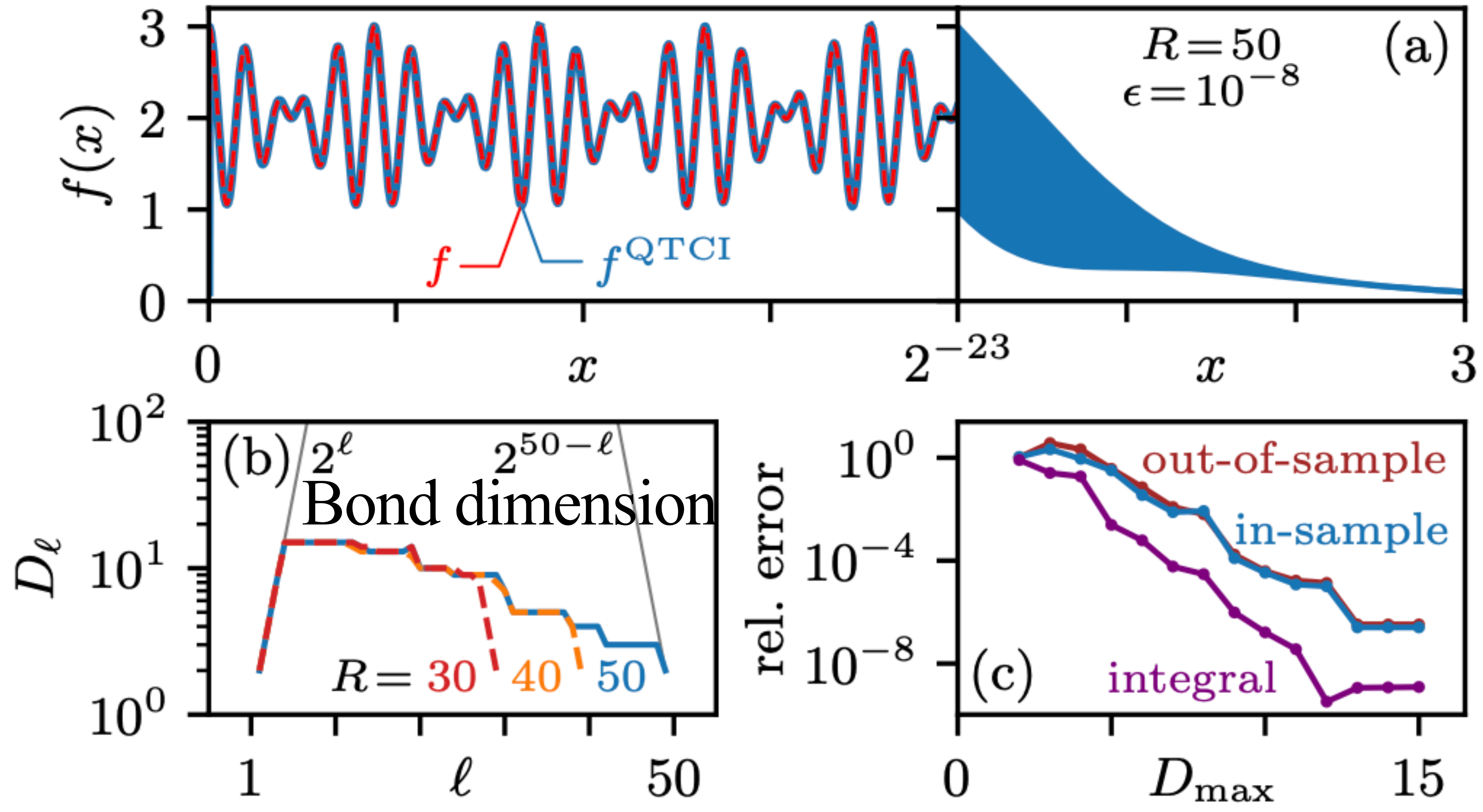
$$f(x) = \cos(\tfrac{x}{B})\cos(\tfrac{x}{4\sqrt{5}B})e^{-x^2} + 2e^{-x} \text{ with } B = 2^{-30} \approx 10^{-9}.$$

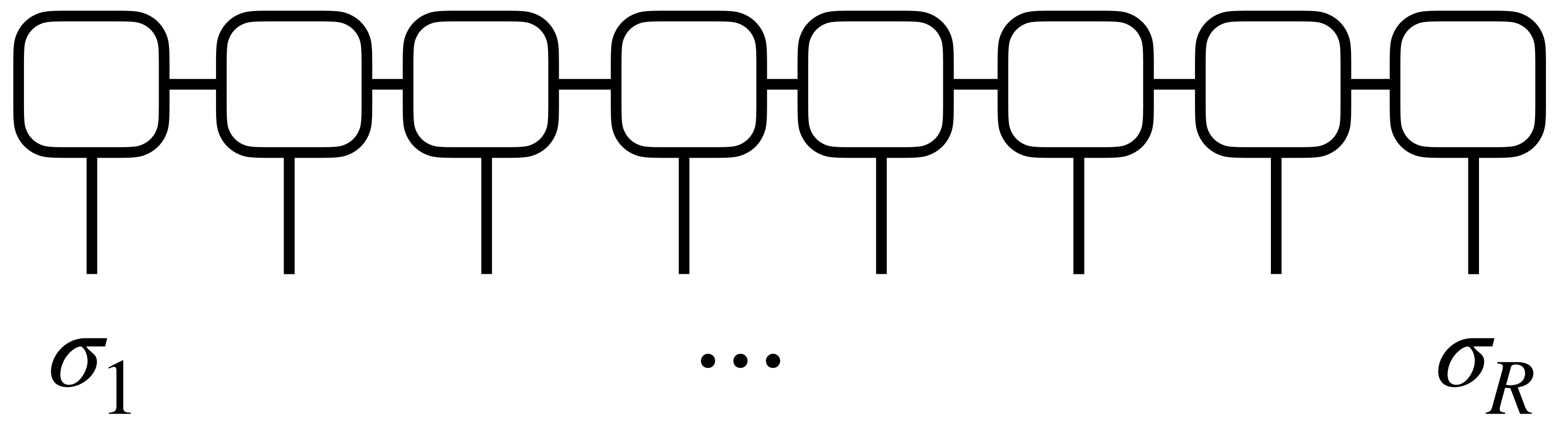
Fast oscillations   Slow decay

Computational complexity ∝ R

8706 samples, i.e., roughly 1 sample per 59000 oscillations.

$R^{50} \approx 10^{15}$ grid points





Bond dimension

Toward efficient quantum-field-theory computation in QTT

BZ integration
M. K. Ritter, Y. N. Fernández, M. Wallerberger, J. von Delft, HS, X. Waintal, PRL **132**, 056501 (2024)

Solving multiorbital impurity models coupled with phonons
H. Ishida, N. Okada, S. Hoshino, and **HS**, arXiv:2405.06440v2

Simulating nonequilibrium dynamics of correlated systems
M. Murray, **HS**, P. Werner, PRB **109**, 165135 (2024)
M. Środa, K. Inayoshi, **HS**, P. Werner, arXiv:2412.14032v1

Solving parquet equations at the two-particle level
S. Rohshap, M. K. Ritter, **HS**, J. von Delft, M. Wallerberger, A. Kauch, arXiv:2410.22975v2

Tensor Cross Interpolation algorithms and software
Y. N. Fernández, M. K. Ritter, M. Jeannin, J.-W. Li, T. Kloss, T. Louvet, S. Terasaki, O. Parcollet, J. von Delft, **HS**, X. Waintal, arXiv:2407.02454v1

Multiorbital electron-phonon model

H. Ishida, N. Okada, S. Hoshino, and **HS**,
arXiv:2405.06440v2

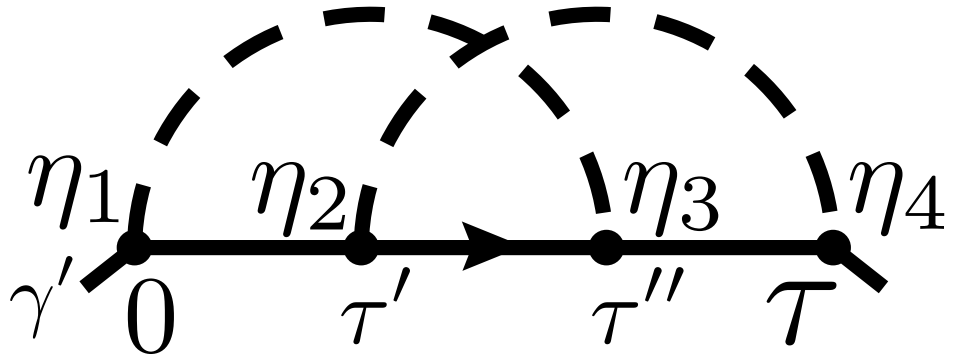
Three orbitals + phonons (for C_{60} lattice)

$$\mathscr{H} = \sum_{ij}\sum_{\gamma\gamma'}\left(t_{ij}^{\gamma\gamma'} - \mu\delta_{ij}\delta_{\gamma\gamma'}\right)c_{i\gamma}^{\dagger}c_{j\gamma'} + \sum_{i\eta}\omega_\eta a_{i\eta}^{\dagger}a_{i\eta} + \sum_{i\eta} I_\eta : T_{i\eta}T_{i\eta} : + \sum_{i\eta} g_\eta \phi_{i\eta} T_{i\eta}$$

i: site
γ, γ': spinorbital
η: phonon

Electron

$$\Sigma^{(2)}_{\gamma\gamma'}(\tau) = \sum_{\substack{\eta_1 \sim \eta_4 \\ \tau', \tau''}}$$



$$f(\gamma, \gamma', \eta_1, \eta_2, \eta_3, \eta_4, \tau, \tau', \tau'')$$

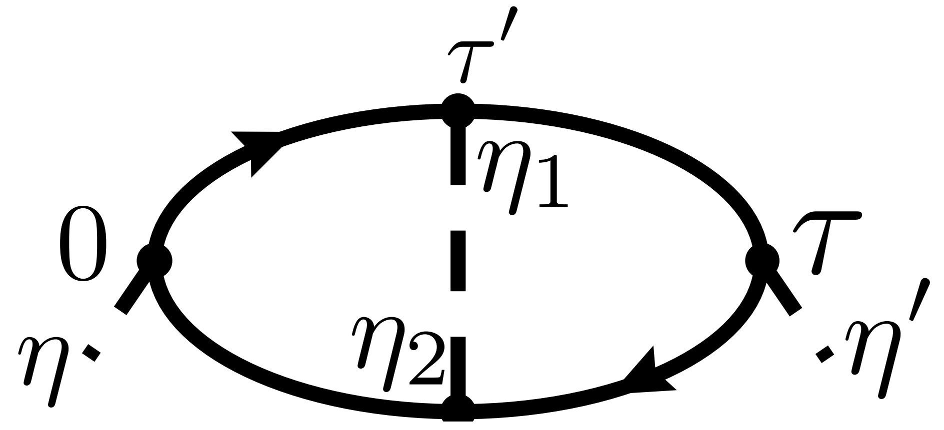
12 12 6 6 6 6 β β β

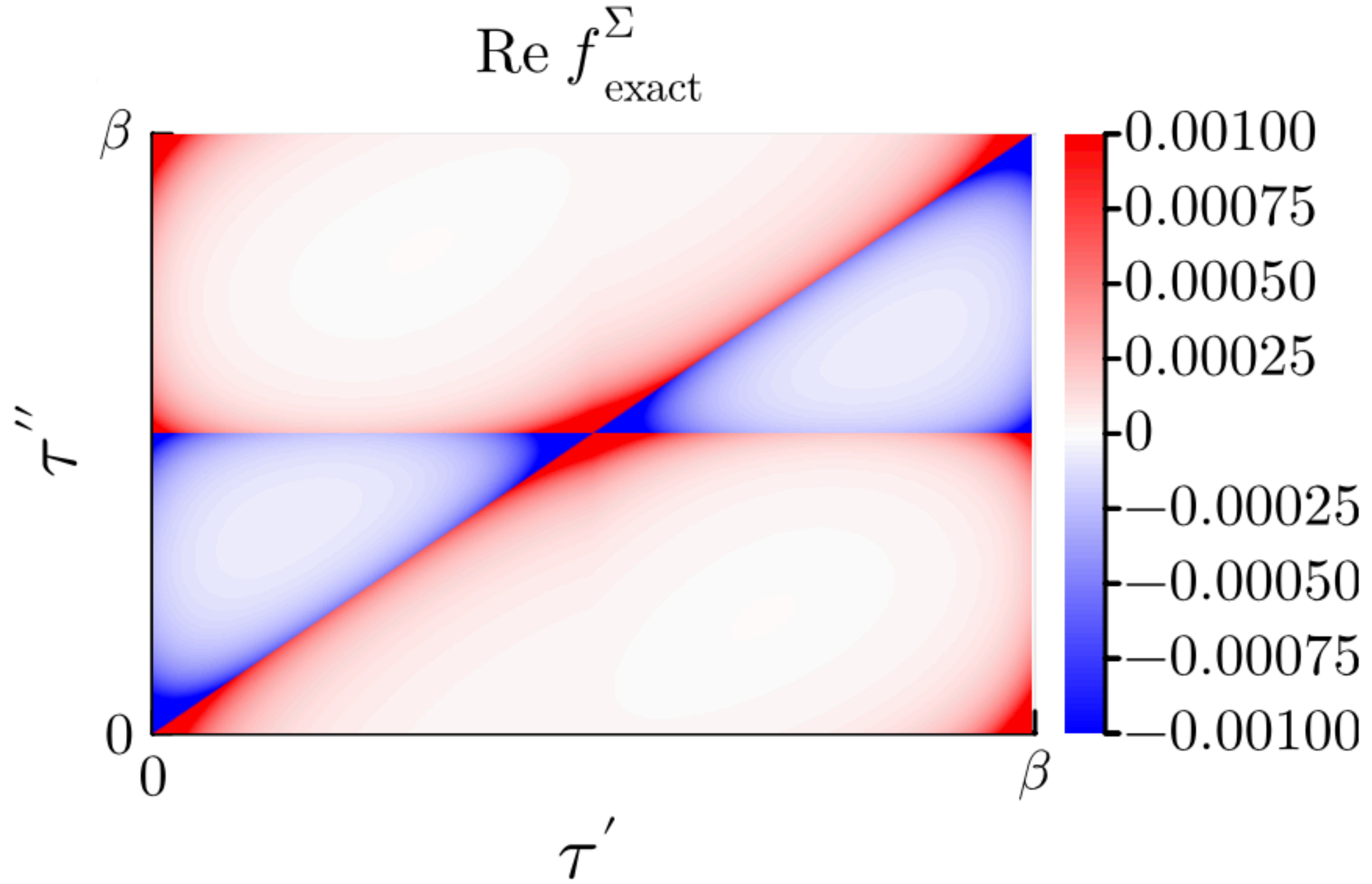
12 = 3 orbital × 2 spins × 2

Nambu modes

Phonon

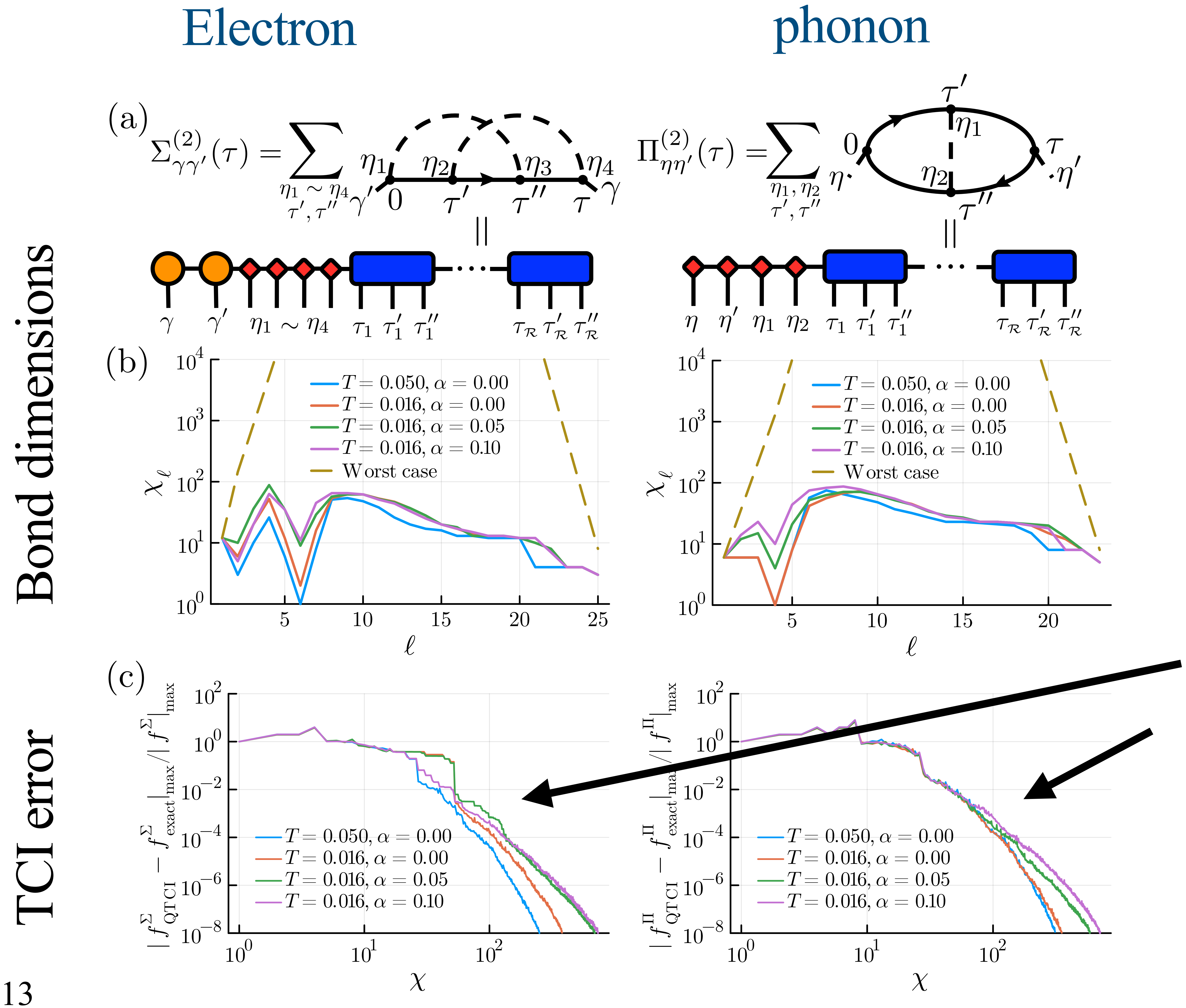
$$\Pi^{(2)}_{\eta\eta'}(\tau) = \sum_{\eta_1, \eta_2}$$

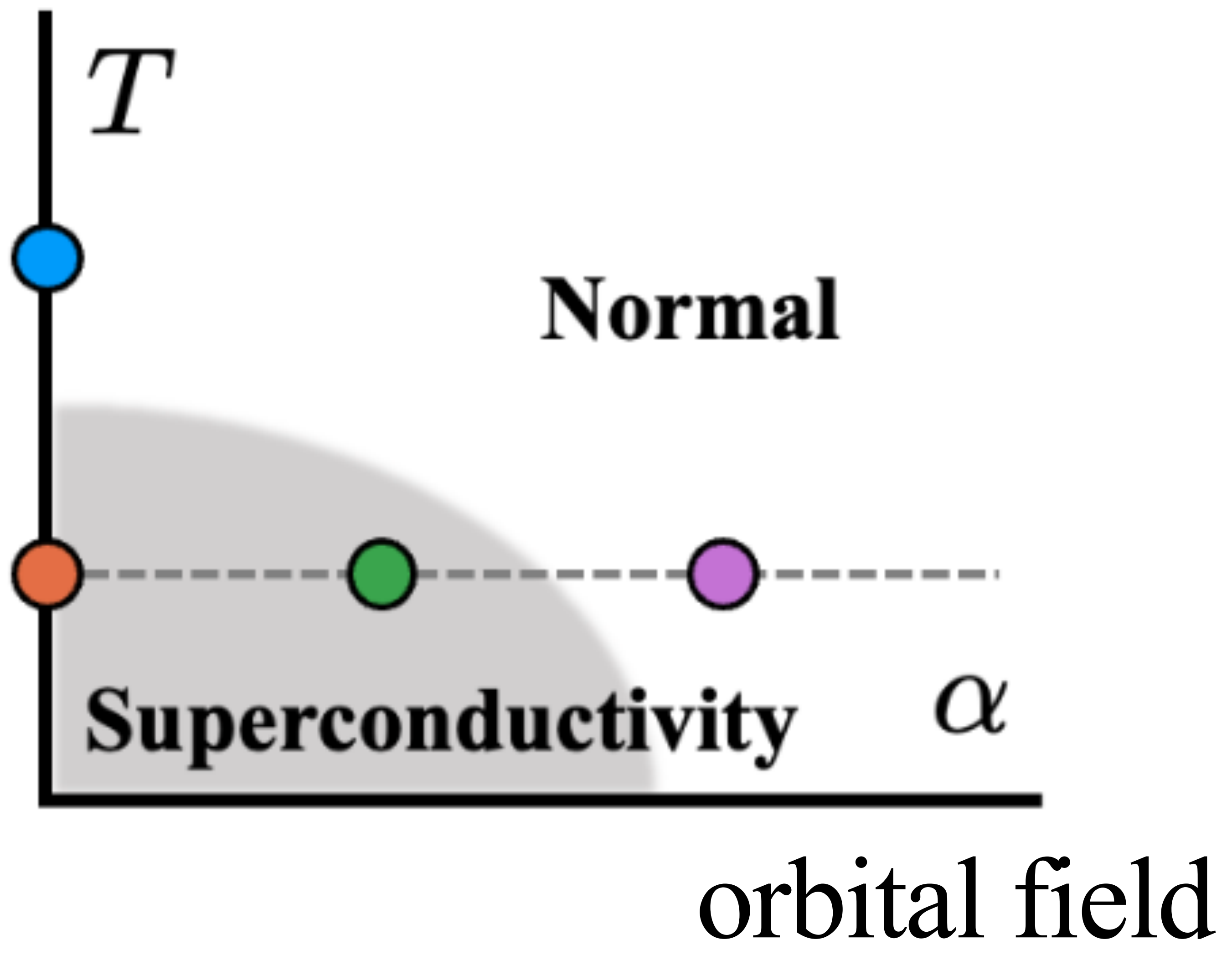




Feynman diagram integration

H. Ishida, N. Okada, S. Hoshino, and **HS**, arXiv:2405.06440v2



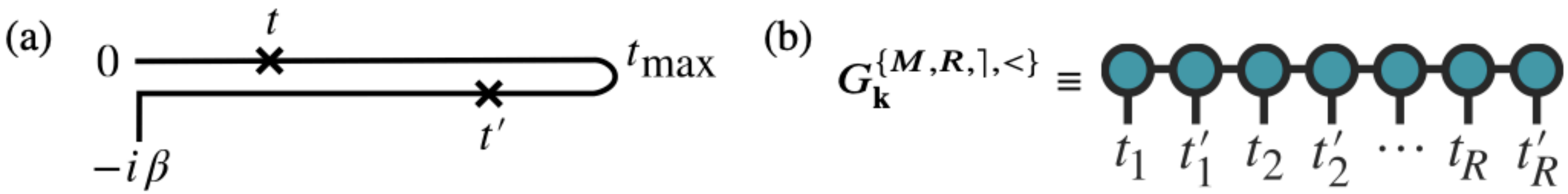


Faster-than-power-law error convergence, unaffected by discontinuity

Future perspectives: higher perturbation orders?

Nonequilibrium *GW* implementation in QTT

M. Środa, K. Inayoshi, **HS**, P. Werner, arXiv:2412.14032v1



Dyson equation solver

$$[1 - G_0\Sigma]G = G_0$$

Convolution, elementwise multiplication

$G(t,t')$

Bosonic part

$$P(t,t') \propto G(t,t')G(t',t)$$

...

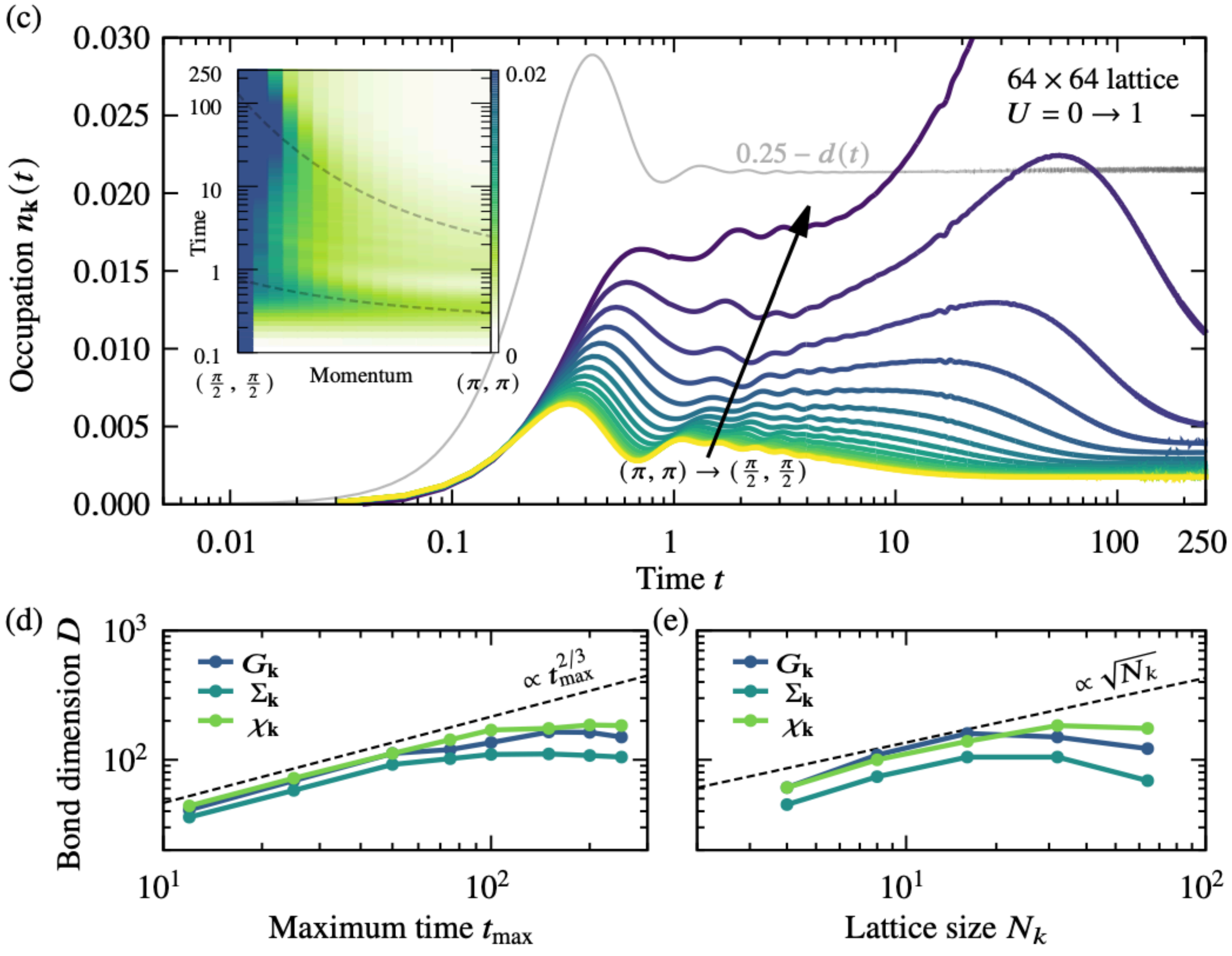
$\Sigma(t,t')$

Impurity solver

$$\Sigma(t,t') \propto G(t,t')\ \delta W(t,t')$$

GW calculations with high k resolution

M. Środa, K. Inayoshi, **HS**, P. Werner, arXiv:2412.14032v1



A dense time grid is too expensive:

$dt = 10^{-2}$, $t_{\max} = 250$, $N_k = 64^3 \to$ 6TB

Huge memory reduction!

QTT time grid: $O(D^2 R N_k) \simeq$ 1GB

D: bond dimension

Outlook: multiorbital, …

Hubbard model, interaction quench $U = 0 \to 1$

tensor4all: open-source libraries and community

https://tensor4all.org/

tensor4all

This website collects information from the tensor4all group which is working on tensor network methods.

Literature

A pedagogical introduction to tensor network methods, which includes an overview of the existing literature and also new algorithms, can be found in:

> Yuriel Núñez Fernández, Marc K. Ritter, Matthieu Jeannin, Jheng-Wei Li, Thomas Kloss, Thibaud Louvet, Satoshi Terasaki, Olivier Parcollet, Jan von Delft, Hiroshi Shinaoka, and Xavier Waintal, arXiv:2407.02454.

Please check the reference page for more information on TCI and quantics tensor trains.

Code

We provide two software libraries that implement algorithms from the above manuscript for computing low-rank tensor representations. The code focuses on recent applications of tensor networks to objects that do not necessarily involve many-body quantum mechanics. It also contain known and new variants of the tensor cross interpolation (TCI) algorithm for unfolding tensors into tensor trains. One code is called Xfac (written in C++ with Python bindings), and a second implementation with similar functionality is based on Julia:

- Xfac (C++ / Python)
- Julia code

maintained by Waintal, von Delft, Shinaoka's groups

- C++/Python/Julia libraries

  Y. Núñez Fernández, M. K. Ritter, M. Jeannin, J.-W. Li, T. Kloss, T. Louvet, S. Terasaki, O. Parcollet, J. von Delft, **HS**, X. Waintal, SciPost Phys. **18**, 104 (2025).
- Mailing list (join us!)
- Monthly online meeting
- Onsite workshop (2025/10/6-10 in Grenoble)

A New Era in Tensor Networks: Exploring Quantics Tensor Networks and Tensor Cross Interpolation

Hiroshi Shinaoka

Lectures at IOP (Feb. 12-14)

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Summary & Outlook

You can find slides online: https://shinaoka.github.io/

QTT: a general framework to exploit scale separation

- ☑ Exponentially fine resolution
- ☑ Multi components (space-time coordinates, spin, orbitals…)
- ☑ Convolution, Fourier transform…
- ☑ Combination with TCI

Outlook: parallelization for HPC, extenstion to tree tensor networks, combination with neural networks?

Hiroshi Shinaoka

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in

杭州量子多体会议本地参会群（340）

Multivariate function

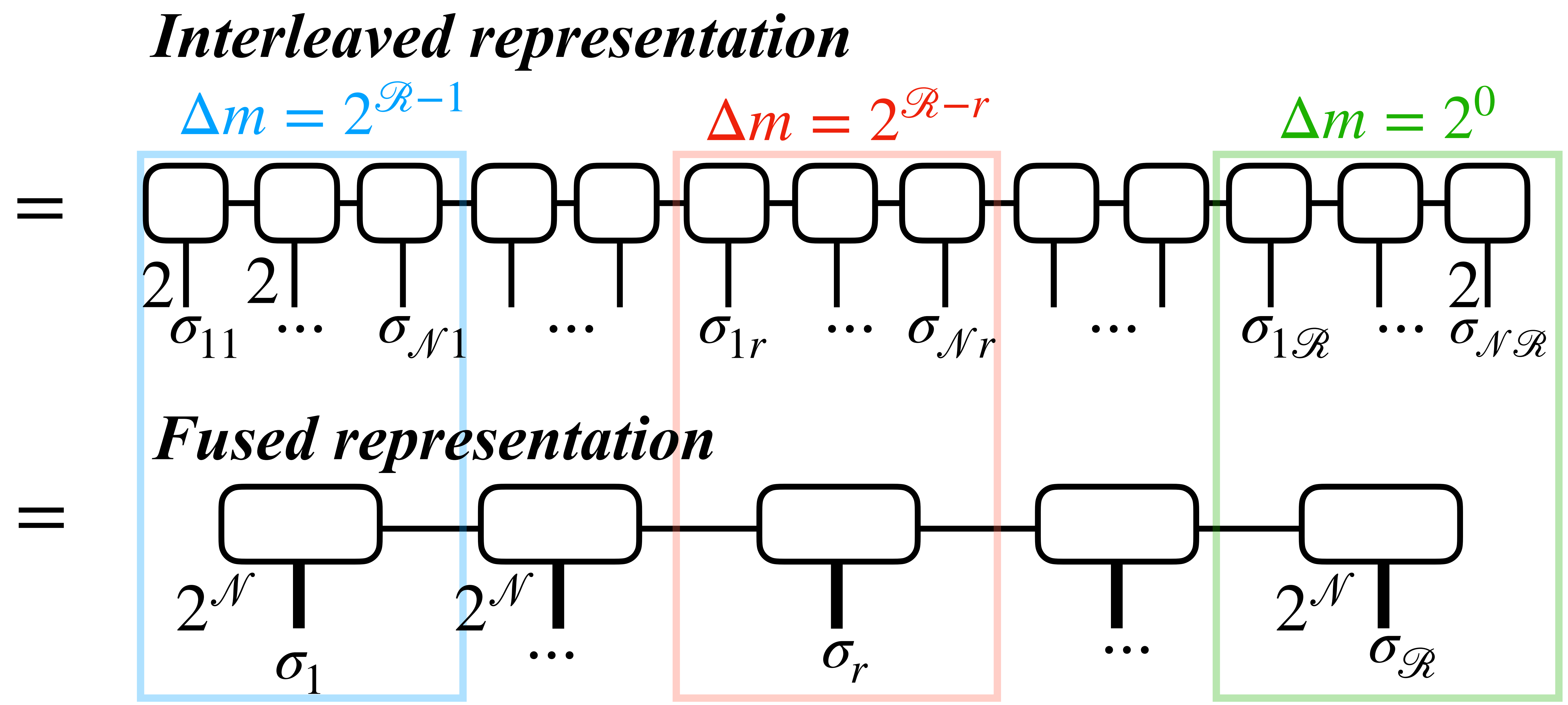
I. V. Oseledets, Doklady Math. **80**, 653 (2009)

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

$\mathcal{N}$-dimensional function $f(x_1, \cdots, x_n, \cdots, x_{\mathcal{N}})$

Binary coding for n-th variable $m_n = (\sigma_{n1} \cdots \sigma_{n\mathcal{R}-1} \sigma_{n\mathcal{R}})_2$

$F_{\sigma_{11} \cdots \sigma_{1\mathcal{R}} \cdots \sigma_{\mathcal{N}1} \cdots \sigma_{\mathcal{N}\mathcal{R}}} =$



$\sigma_r \equiv (\sigma_{1r} \cdots \sigma_{\mathcal{N}r})$

Degrees of freedom at the same length scale are usually highly entangled.

Compressible functions

Exponential function

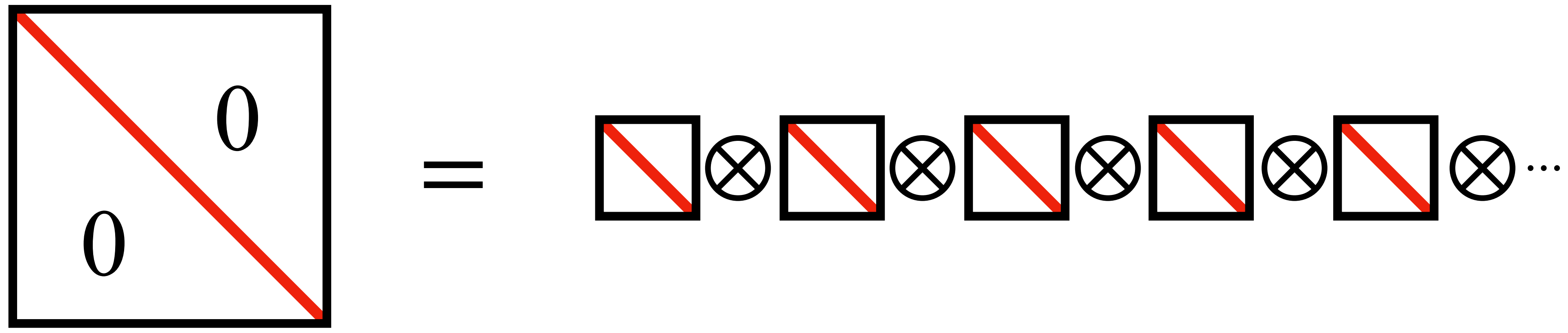
$$f(x) = e^{-x} = e^{-x_1/2} e^{-x_2/2^2} \cdots e^{-x_n/2^n} \cdots \quad \chi = 1$$

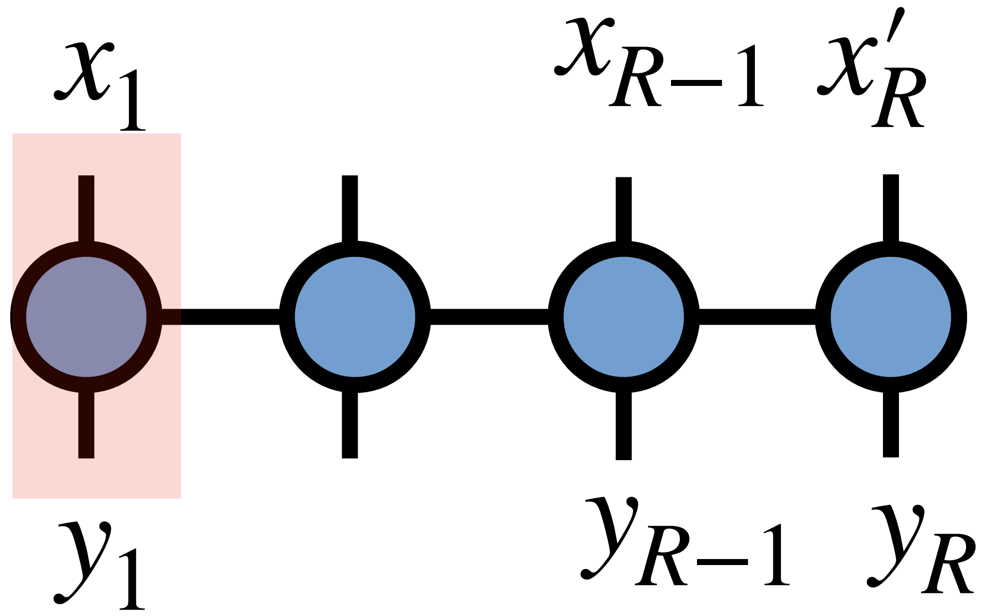
$$x = (0.x_1 x_2 \cdots x_n \cdots)_2 \in [0,1)$$

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.

Identity matrix

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





- Representation of Continuous Functions: https://tensornetwork.org/functions/ by Miles Stoudenmire
- B. N. Khoromskij, Tensor Numerical Methods in Scientific Computing, doi:10.1515/978311036591

Less compressible functions

χ increases exponentially with $\mathscr{R}$.

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

Discontinuity on curved boundary

∵ # of linearly independent patches increases exponentially.