Learning Feynman Diagrams with Tensor Trains

Olivier Parcollet

FLATIRON INSTITUTE
Center for Computational Quantum Physics

Precision Many-Body Physics
Collège de France, June 14th 2023

Phys Rev X 12, 041018 (2022)

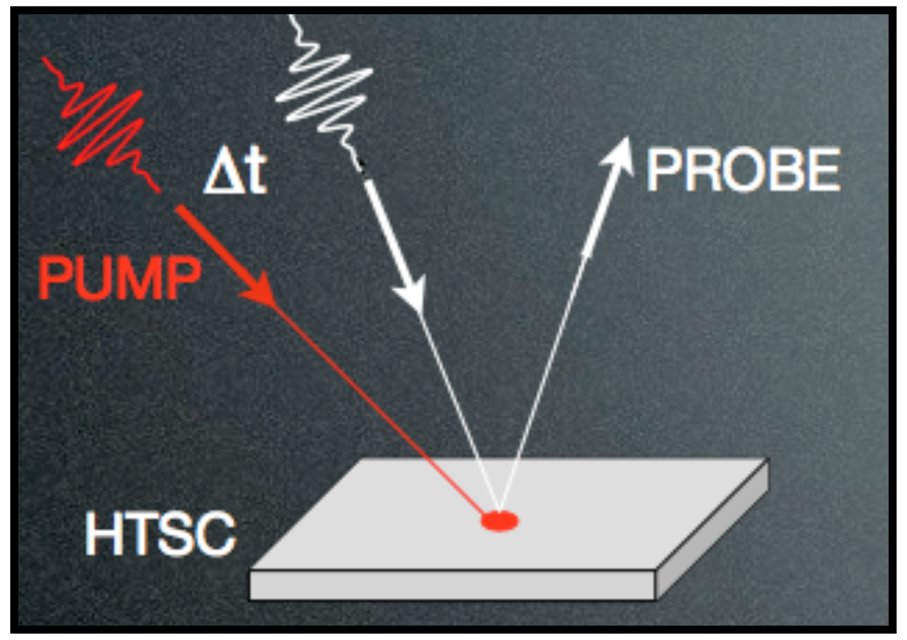
Collaborators : Y. Nuñez-Fernandez, M. Jeannin, Ph. Dumitrescu, T. Kloss, J. Kaye, X. Waintal

Outline:
Tensor Train Diagrammatics

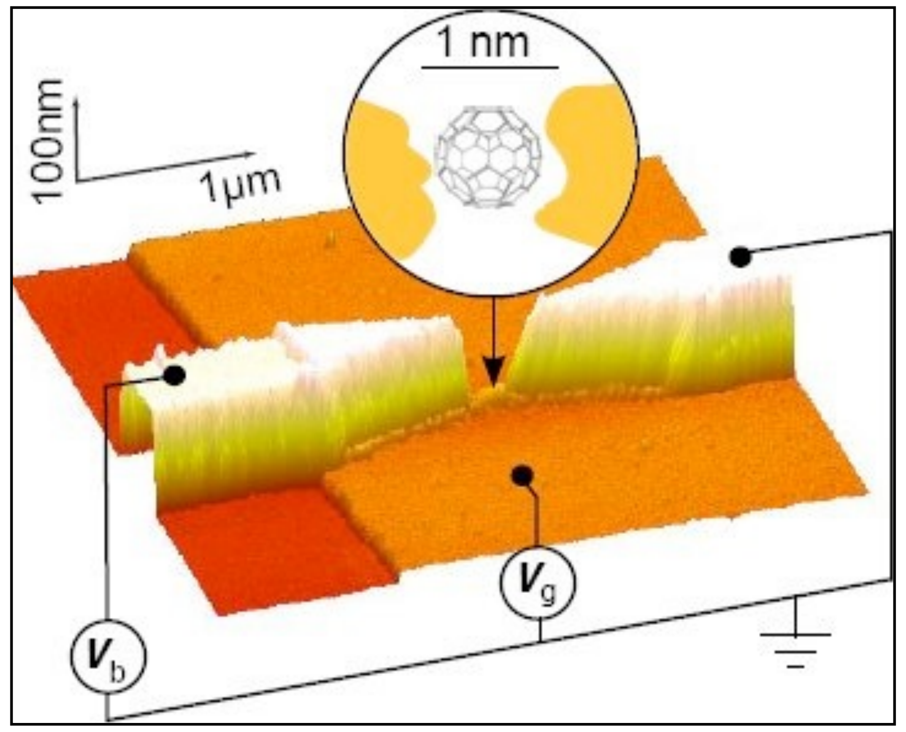
- A diagrammatic approach for out of equilibrium interacting quantum systems.
- Tensor Cross Interpolation
  A tensor decomposition technique for high dimensional integration.

Out of equilibrium & strong correlations

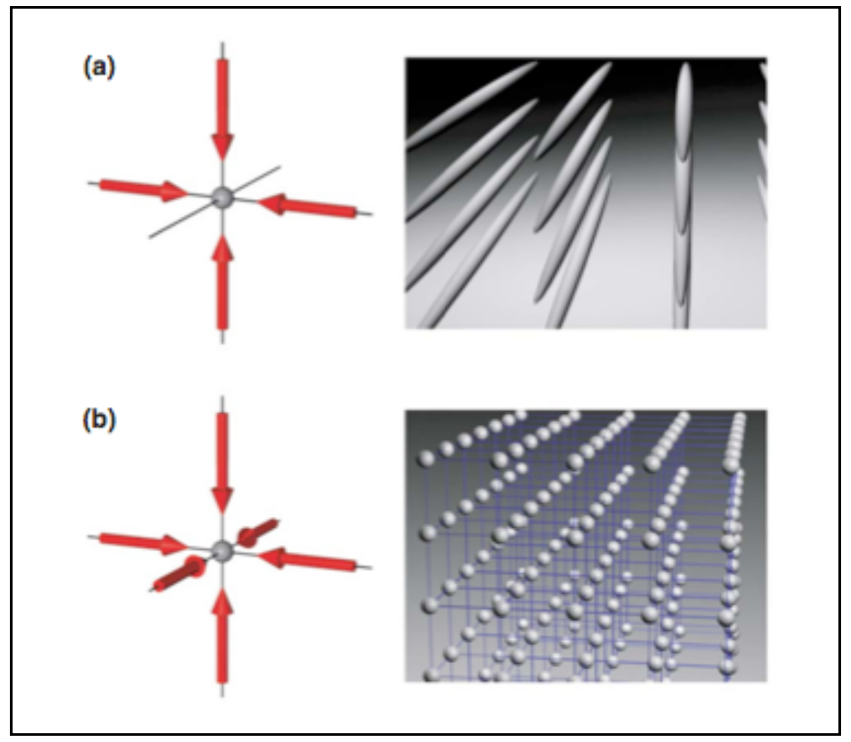
- Many experiments : Pump probe, quantum dots, ultra-cold atoms, cavities.



Pump probe



Nano-electronics

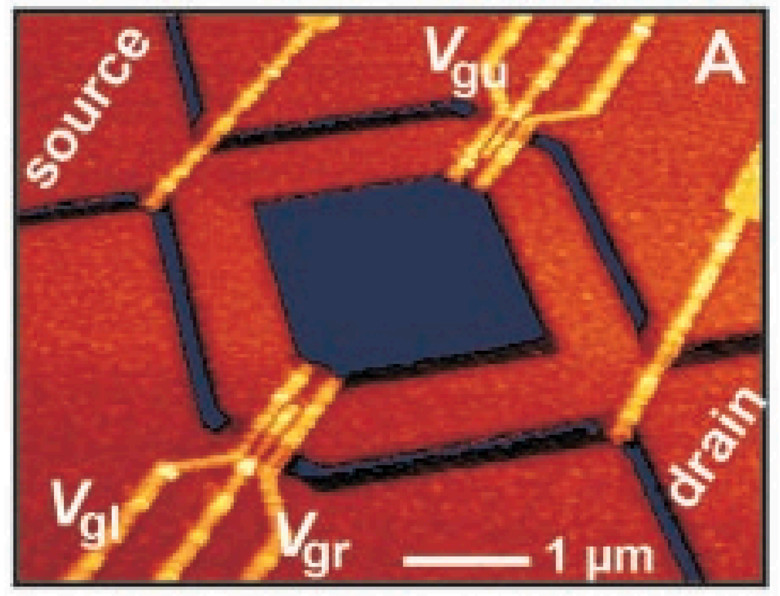


Ultra-cold atoms

- Computational physics challenge :
  - Exact methods for out of equilibrium systems, at strong coupling
  - Control, speed and precision
  - Long time (after quench), steady state. Resolve various energy/time scales.

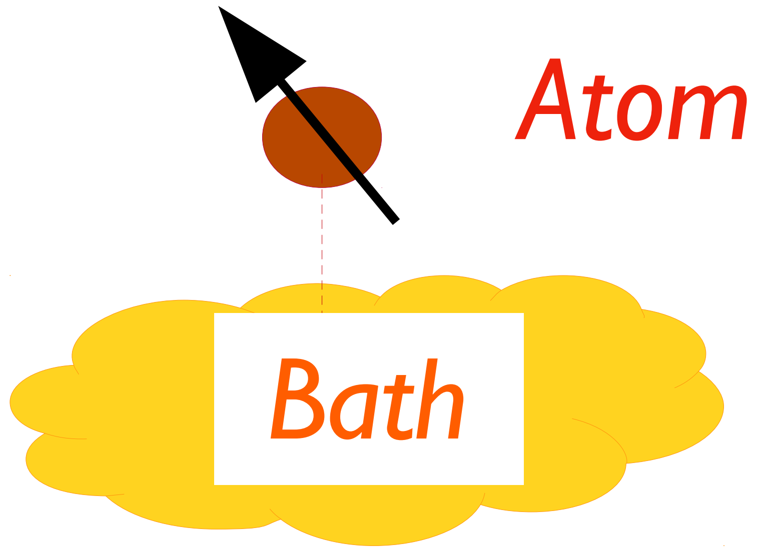
Models

Quantum dots
Quantum impurity models



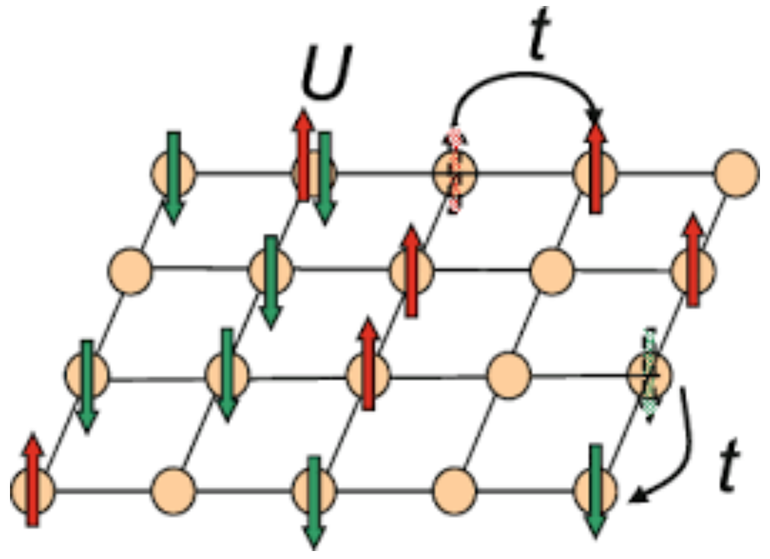
- High precision benchmark in equilibrium (Bethe Ansatz)
- Strong coupling : Kondo effect
  L .Glazman et al., P. Lee 1988.
  D. Goldhaber-Gordon, 1998

Quantum embeddings



- Out of equilibrium solvers.

Lattice models



- Non equilibrium. Transport. Real time dynamics.

Perturbative series

- In equilibrium, Diagrammatic Quantum Monte Carlo

From Prokofiev, Svistunov 98,
Many works in equilibrium
Cf F. Simkovic's talk.

- In this talk: real time, out of equilibrium, with Schwinger-Keldysh diagrammatics.

Profumo, Messio, Parcollet, Waintal PRB (2015) *Bertrand, Florens, Parcollet, Waintal PRX 9, 041008 (2019)*

$$Q(t, U) = \sum_{n=0}^{K} Q_n(t) U^n \qquad K \approx 10 - 20$$

Time *Interaction*

- Works even at long time, even in strong coupling regime (e.g. Kondo effect)

1. How to compute $Q_n(t)$?
2. How to sum the perturbative series ?

Perturbative series

Profumo, Messio, Parcollet, Waintal (2015)

Bertrand, Florens, Parcollet, Waintal PRX 9, 041008 (2019)

- Q_n is a n-dimensional integral.

$$Q(t, U) = \sum_{n=0}^{K} Q_n(t) U^n \qquad Q_n(t) = \int du_1 \ldots du_n \;\; q_n(t, u_1, \ldots, u_n)$$

Sum of all Feynman diagrams at order n in $O(2^n)$

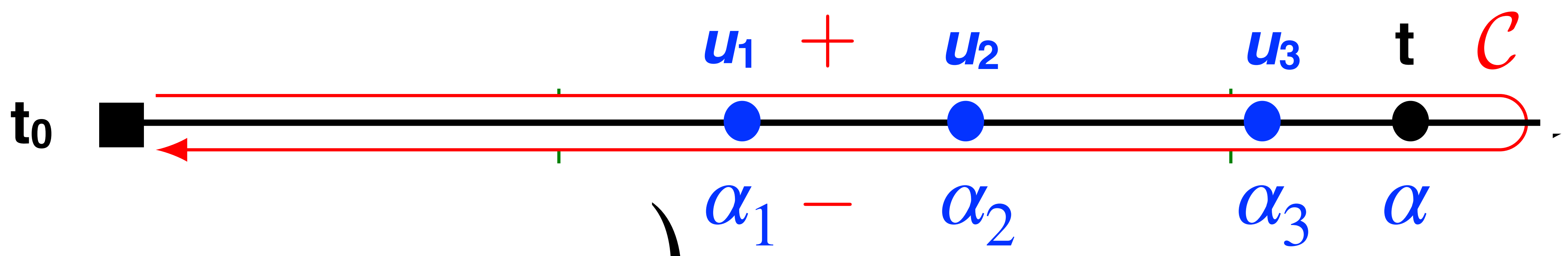
- Sum the perturbative series
  - At finite time t/volume, the series is convergent for all U
  - In steady state $t \to \infty$, finite radius of convergence in U
    - Beyond weak coupling, use conformal change of variable in the U plane.
    - Change the starting point of the expansion (quadratic counter-terms)

$Q_n(t)$: a n-dimensional integral

- Schwinger-Keldysh formalism

Switch on interaction

Times u_i
Keldysh indices $\alpha = \pm 1$



$$Q_n(t) = \frac{1}{n!} \boxed{\int_{t_0}^{\infty} du_1 \ldots du_n} \left(\sum_{\substack{\alpha_1 = \pm 1 \\ \ldots \\ \alpha_n = \pm 1}} \left(\prod_{i=1}^{n} \alpha_i \right) \det_{0 \le i,j \le n} \left[g_{\alpha_i \alpha_j}(u_i - u_j) \right] \right)$$

Monte Carlo or Tensor network …

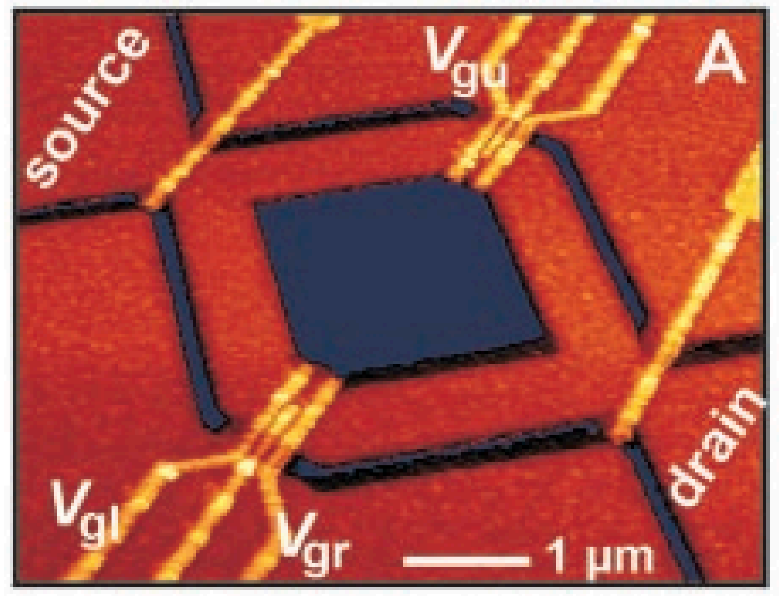
$\equiv q_n(t, u_1, \ldots, u_n)$

Green function in the non interacting case $U = 0$

- Feynman diagrams explicitly summed by the determinants (Wick theorem).
- q_n costs $O(2^n)$ to evaluate. Typically, 10-15 orders.
- Equilibrium/steady state = long time limit $t \to \infty$ is easy. Vacuum diagram cancellations.

Quantum dot
A sample of results

Anderson model



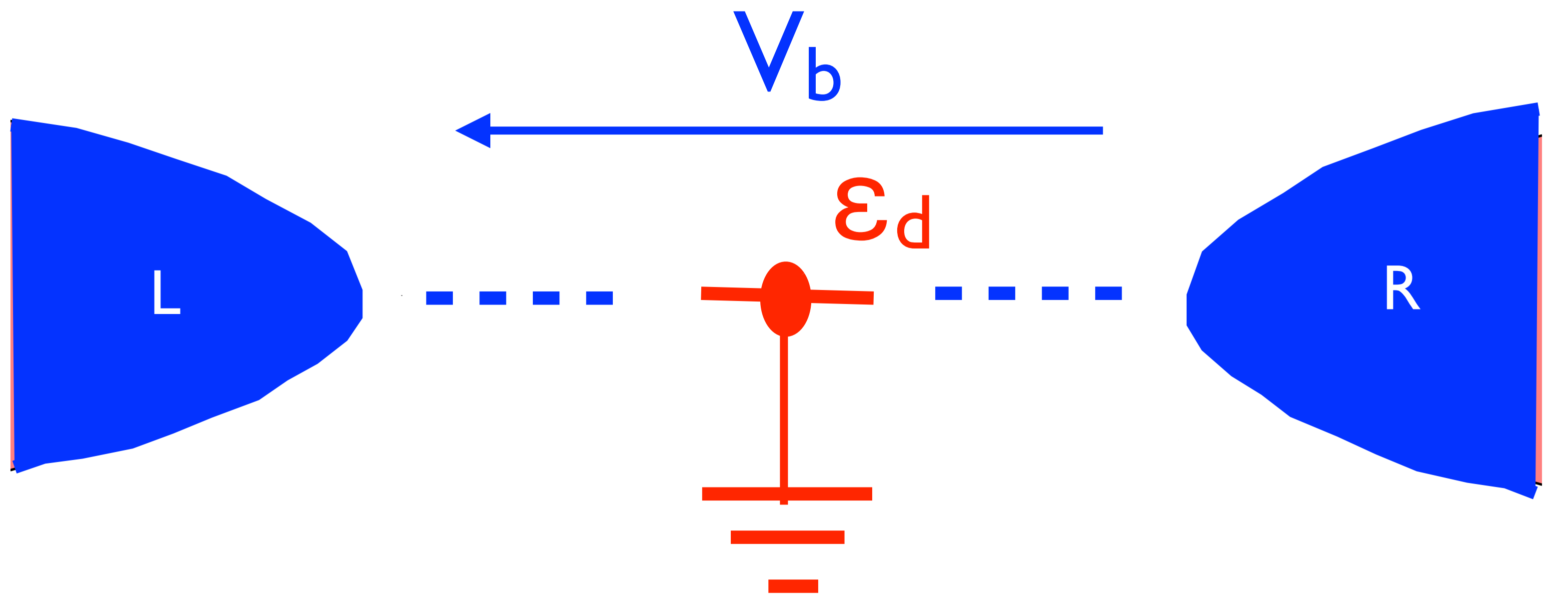
- Two leads (L, R).

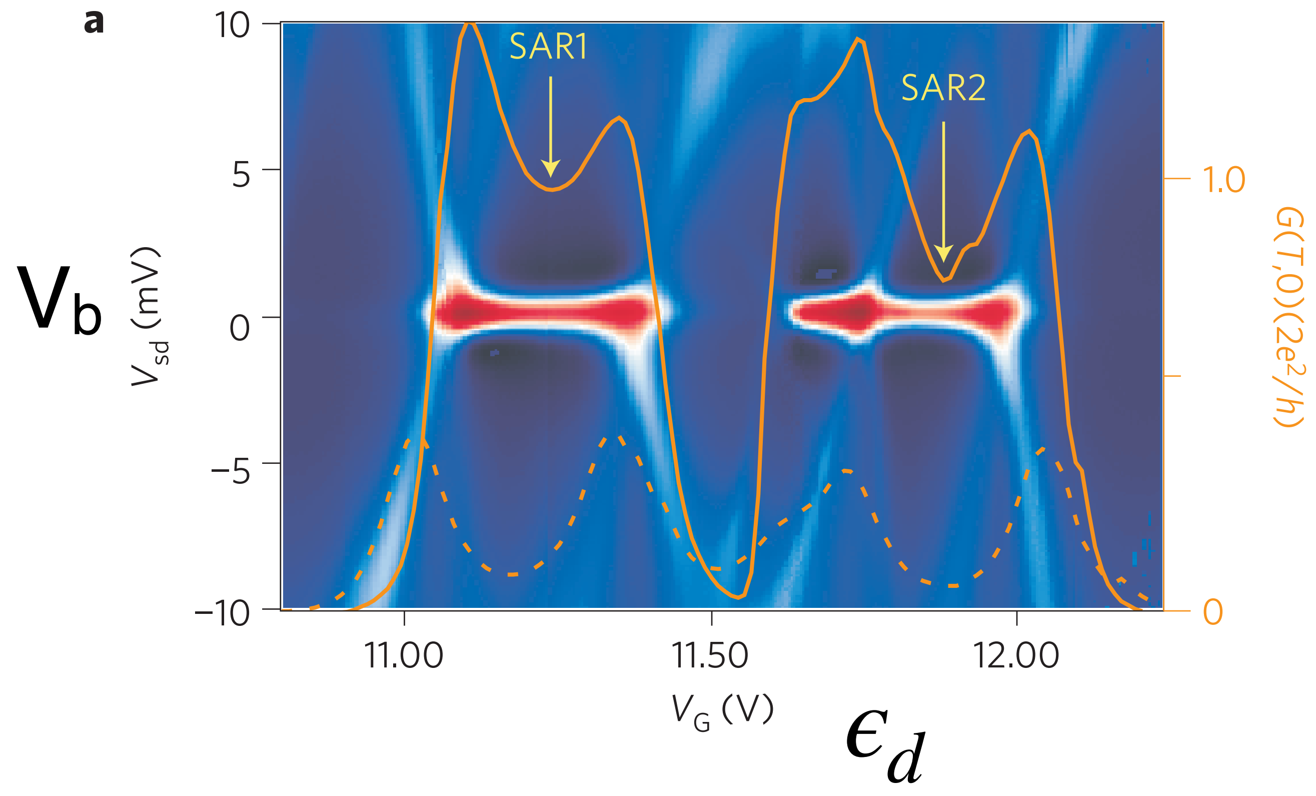
Bath   *Local orbital*   *Hybridization*

$$H = \sum_{\substack{k\sigma \\ \alpha = L,R}} \varepsilon_{k\alpha} c^\dagger_{k\sigma\alpha} c_{k\sigma\alpha} + \sum_\sigma \varepsilon_d d^\dagger_\sigma d_\sigma + U n_{d\uparrow} n_{d\downarrow} + \sum_{\substack{k\sigma \\ \alpha = L,R}} g_{k\sigma\alpha} (c^\dagger_{k\sigma\alpha} d_\sigma + h.c.)$$

Level width at U=0

$$\Gamma = \pi \rho_{E_F} g^2$$





- Questions : Spectral function ? Kondo temperature ? Current ?

We want a precise solution, at low temperature, any V_b, in steady state

Experiment : T. Delattre et al. Nat. Phys. 208 (2009)

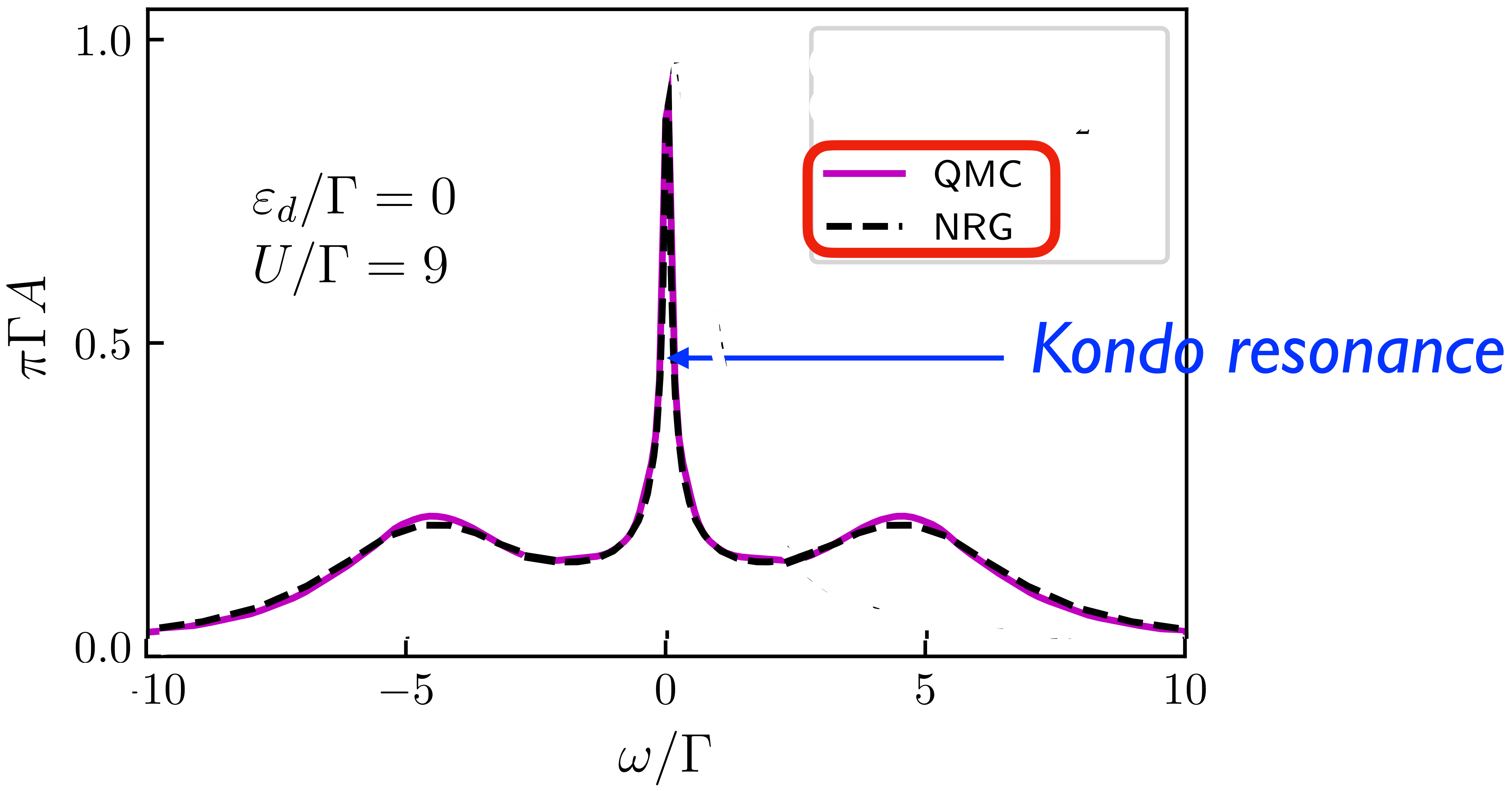
Kondo effect in equilibrium

$$A(\omega) = -\frac{1}{\pi} ImG^R(\omega)$$

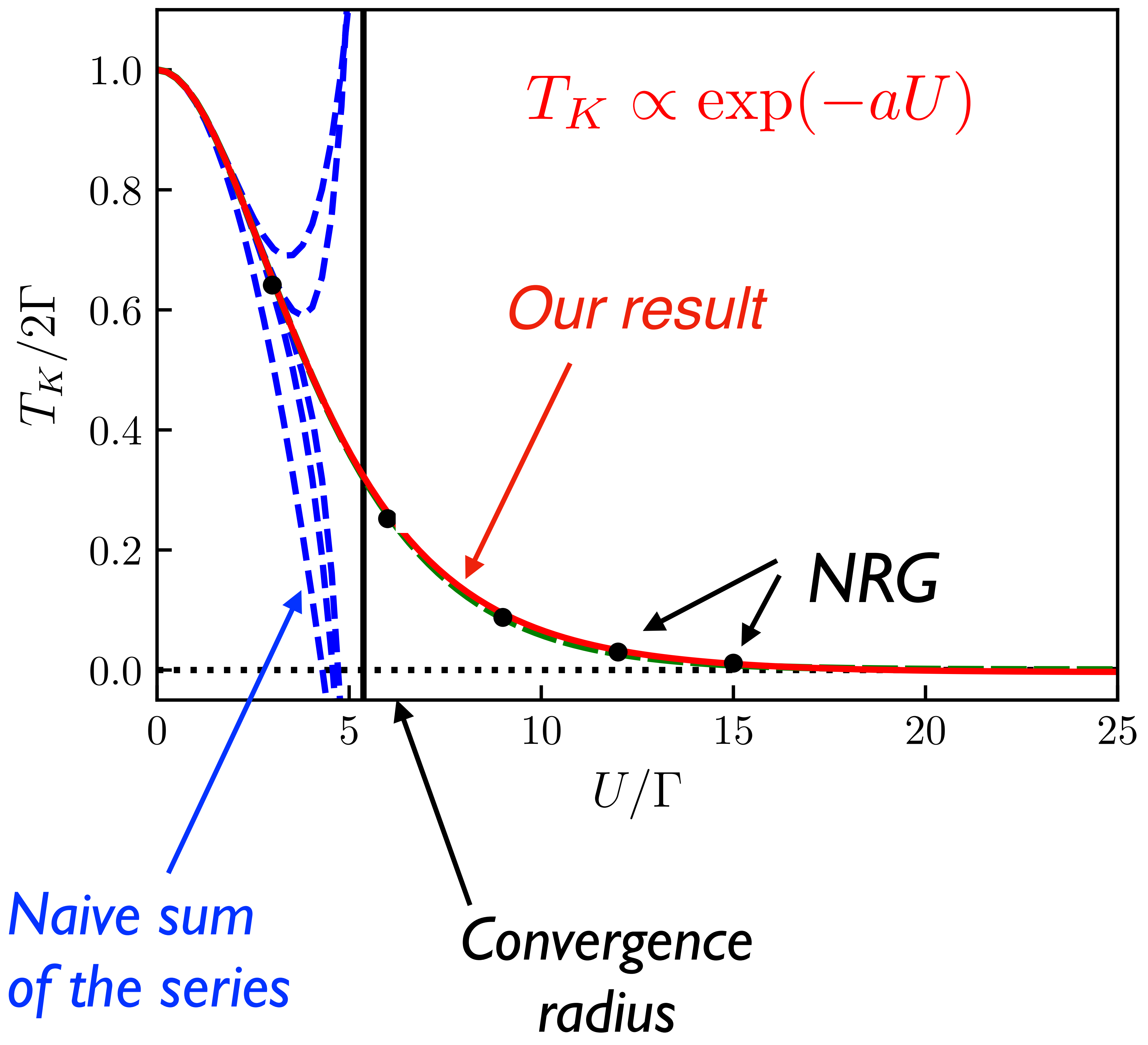
Bertrand et al. Phys. Rev. X (2019)

Spectral function of the dot

Kondo temperature $T_K(U) \equiv \frac{2\Gamma}{1 - \partial_\omega \mathrm{Re}\Sigma^R(U,\omega)\big|_{\omega=0}}$



$$T = 10^{-4}\Gamma$$

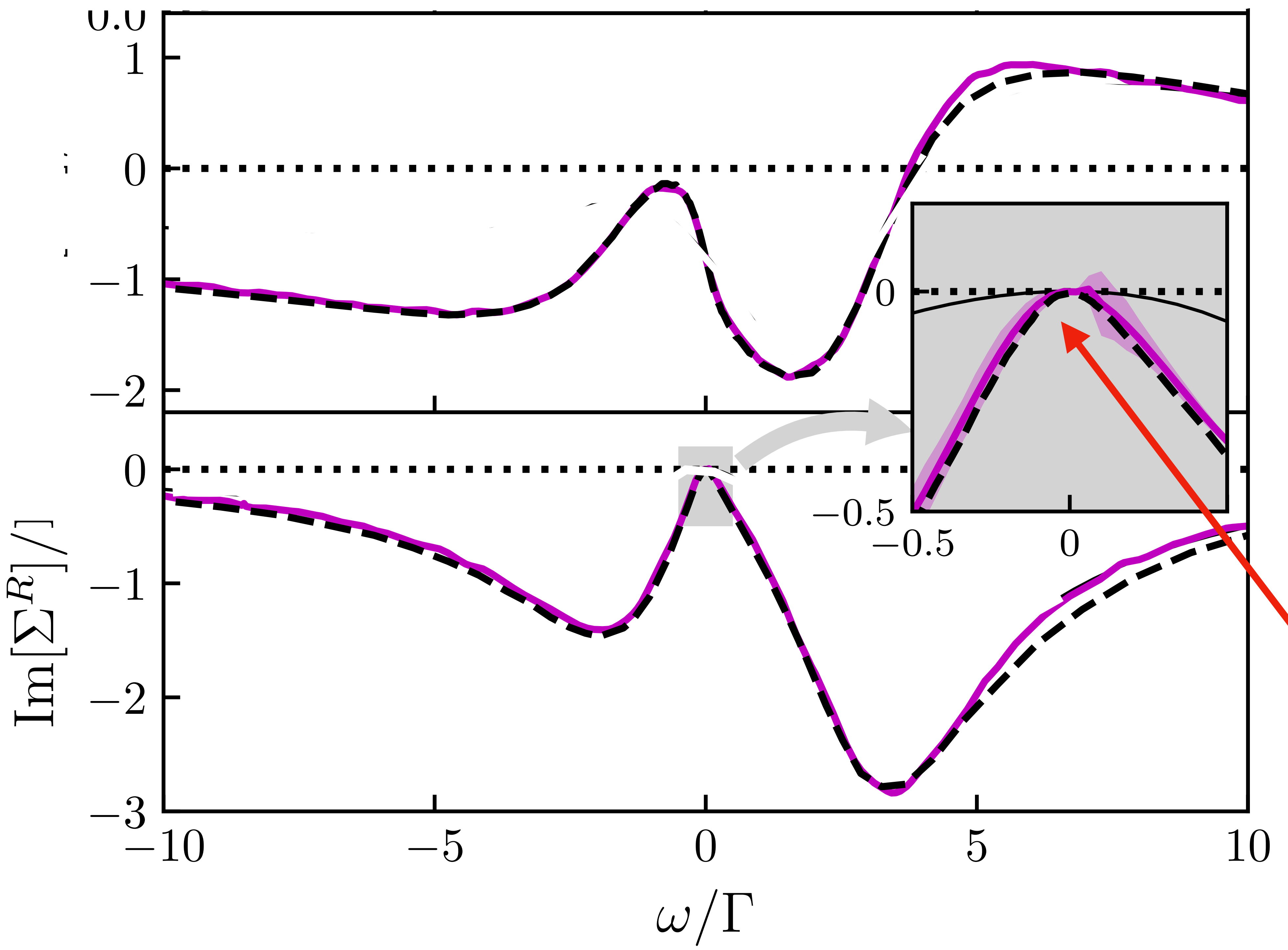


Fermi liquid self-energy at low energy

C. Bertrand et al.
Phys. Rev. X 9, 041008 (2019)

$Re\Sigma^R(\omega)/\Gamma$

$Im\Sigma^R(\omega)/\Gamma$



Real time QMC

NRG benchmark

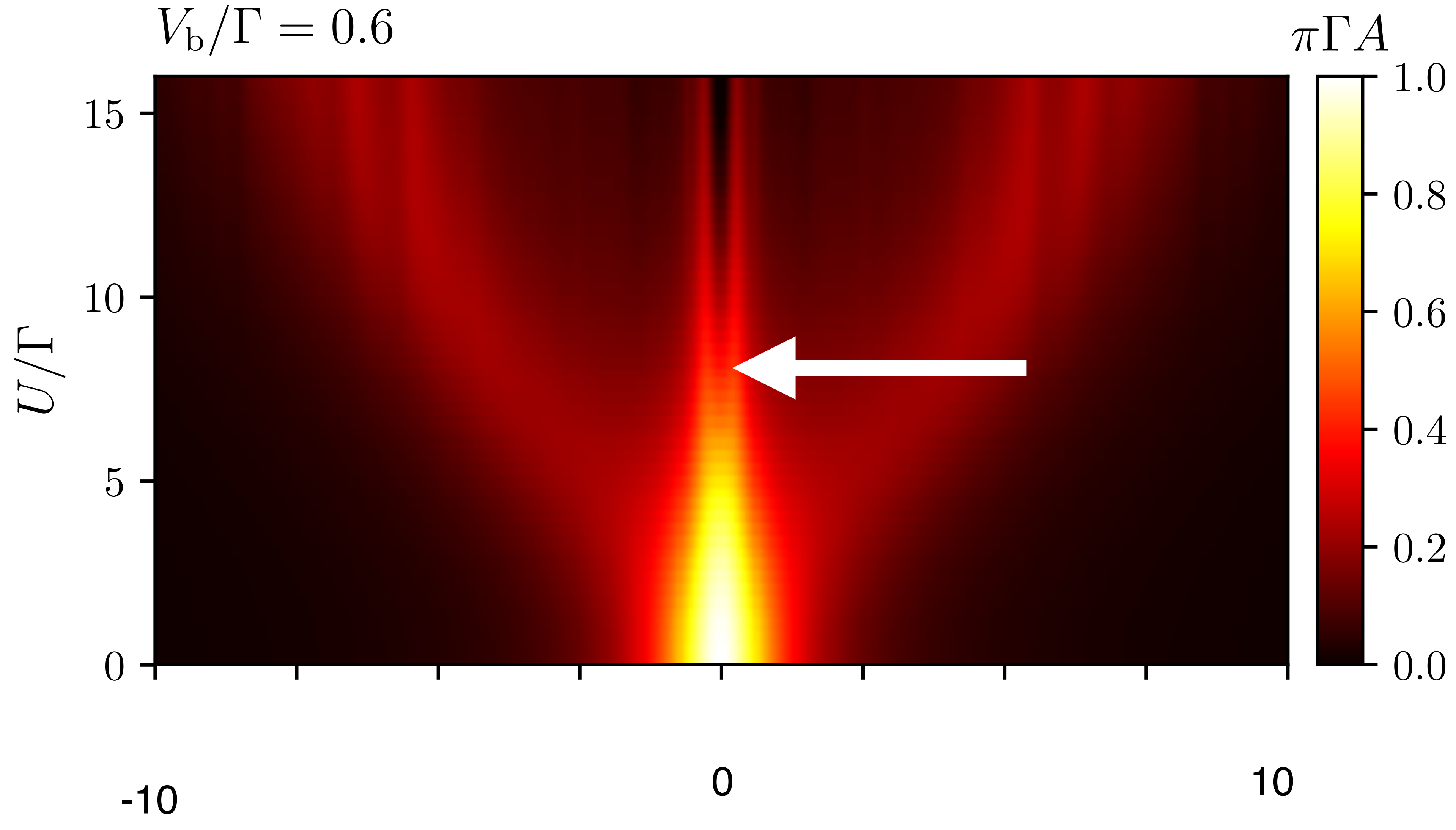
$\epsilon_d/\Gamma = 1$ $\quad T = 0$

$U/\Gamma = 6$

$Im\Sigma(\omega) \sim \omega^2$

Out of equilibrium

Kondo resonance



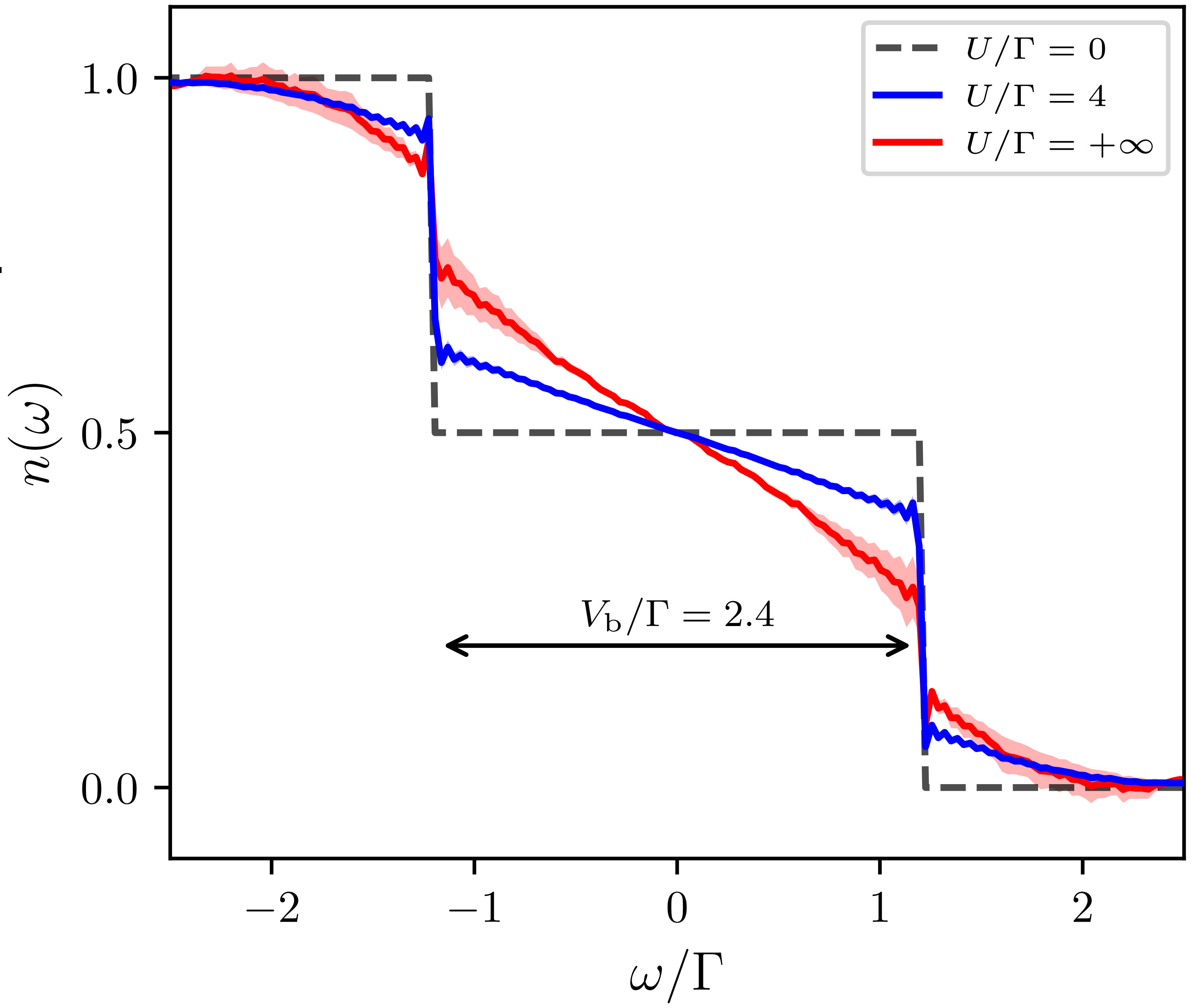
T = Γ/50

- Split by voltage bias V_b
- One calculation, all U

Dot non-thermal distribution function

at $T = 0$ with voltage V_b

$$n(\omega) \equiv \frac{G^<(\omega)}{2\pi i A(\omega)}$$

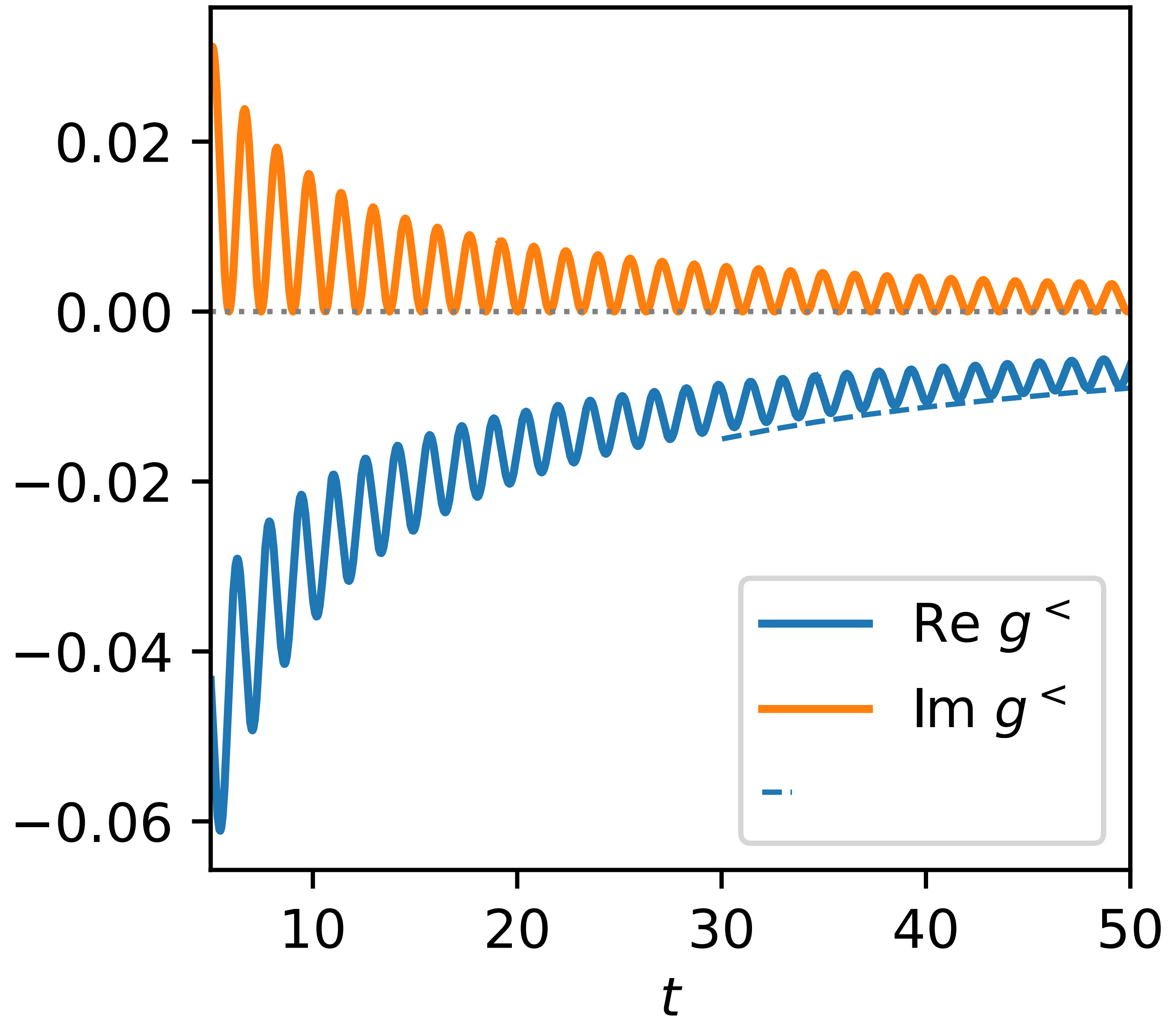


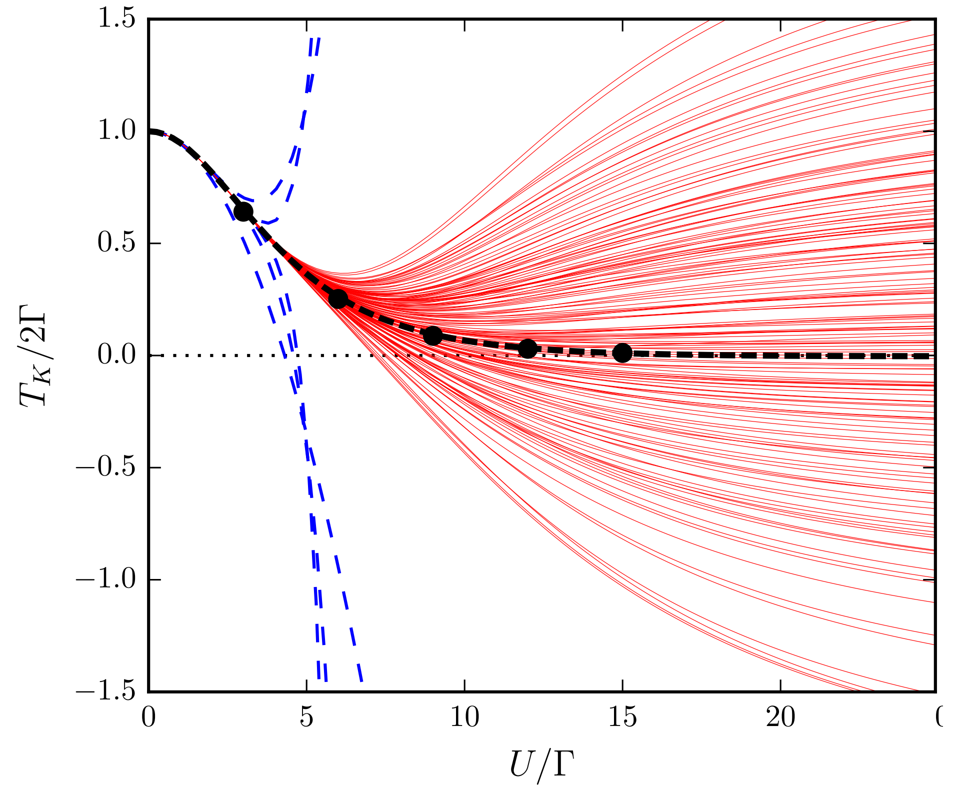
Bertrand et al. Phys. Rev. X (2019)

Limitations of Monte Carlo

- <u>Speed</u>. Error in MC is $O(1/\sqrt{N})$
- <u>Sign problem</u>. Very oscillating integrals in some regimes.
- <u>Precision</u> on expansion coefficients Q_n
  Resummation techniques can amplify noise.

Bare local Green function vs t (Hubbard lattice, T=0)





- In this case, we used a non perturbative information

$$T_K(U) \underset{U\to\infty}{\to} 0$$

to constraint the series summation (Bayesian inference technique)

Using Tensor Networks to integrate in large dimensions

Large dimension integrals

- Large dimension integral or sum ($n \geq 10$)

$$\int dx_1 \ldots dx_n \; f(x_1, \ldots, x_n) \qquad\qquad \sum_{i_1=1}^{d} \cdots \sum_{i_n=1}^{d} f_{i_1,\ldots,i_n}$$

- Discretize the integral (e.g. Legendre grid) with d points : discrete x_i
- Curse of dimensionality : a priori $O(d^n)$.
- An ubiquitous problem in the quantum many-body problems, e.g.
  - Diagrammatics (real time, imaginary time).
  - Partition functions.

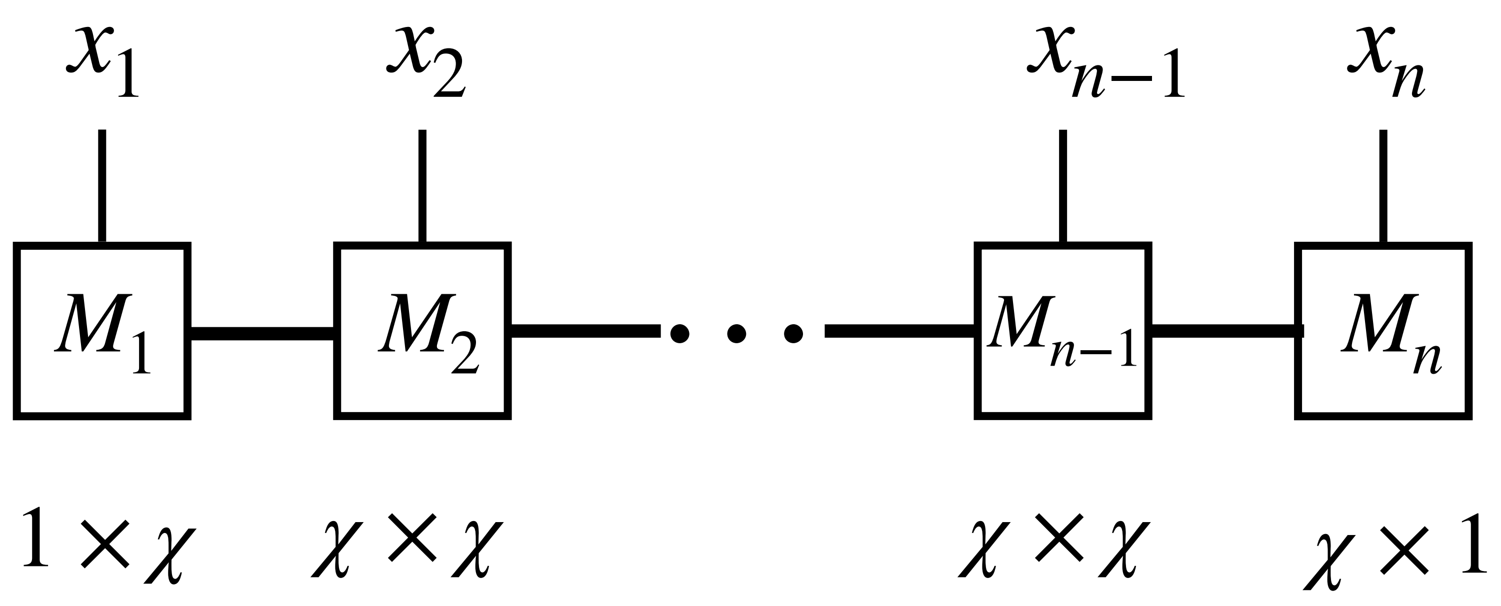
Main idea : compress to integrate

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

$$\int dx_1 \ldots dx_n \; f(x_1, \ldots, x_n)$$

- <u>If</u> *f* can be written as a Matrix Product State (MPS) …

$$f(x_1, \ldots, x_n) \approx M_1(x_1) \ldots M_n(x_n) \qquad =$$

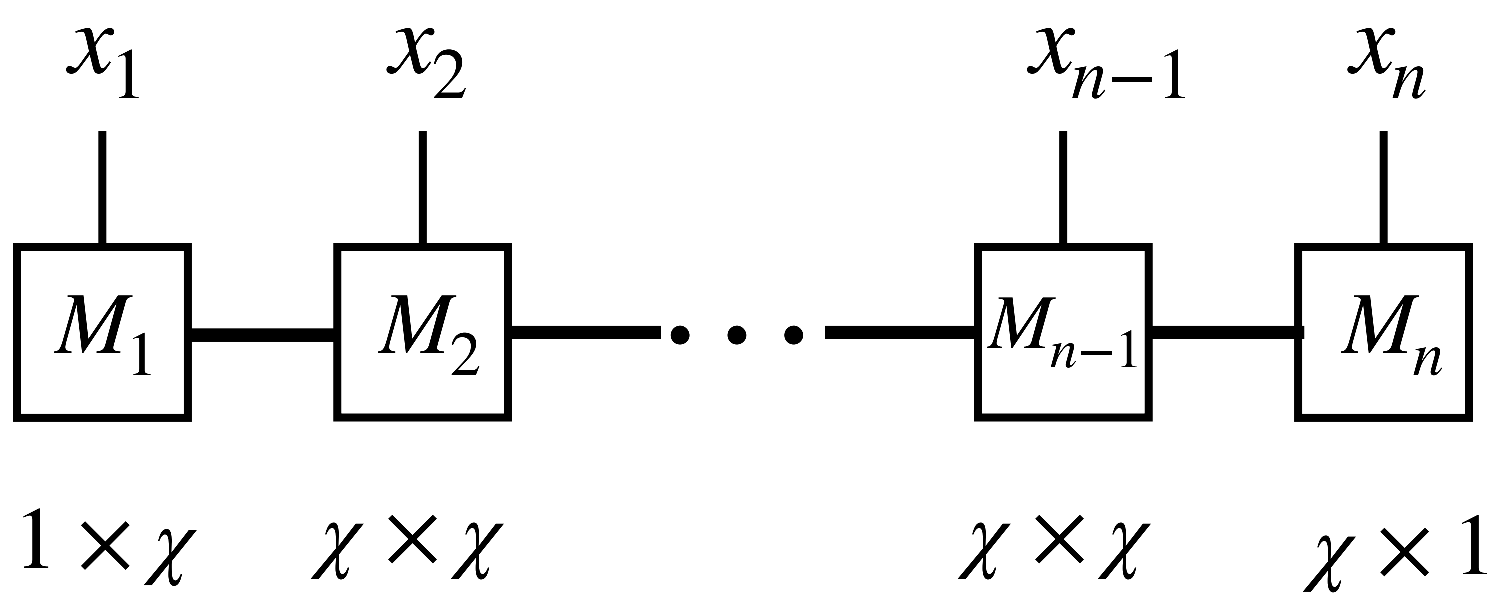


- with an error ε decreasing quickly with the rank χ (*ε-factorizable*) …
- then integration is reduced to 1d integrals. Almost separated variables.

$$\int dx_1 \ldots dx_n \; f(x_1, \ldots, x_n) \approx \left(\int dx_1 M_1(x_1) \right) \ldots \left(\int dx_n M_n(x_n) \right)$$

MPS compression

$$f(x_1, \ldots, x_n) \approx M_1(x_1) \ldots M_n(x_n) \quad = $$



- Does our function of interest have this form ? If yes, how to find M_i ?
- We use a <u>rank revealing</u> technique : Tensor Cross Interpolation (TCI)
- Goals :
  - Minimal number of evaluations of f.
  - A reliable error estimate.

- *Oseledets et al (2010)*
- *S. Dolgov and D. Savostyanov, (2020)*

q_n is ε-factorizable !

$$Q_n(t) = \int_{t_0}^{\infty} du_1 \ldots du_n \;\; q_n(t, u_1, \ldots, u_n)$$

$$q_n(t, u_1, \ldots, u_n) = \frac{1}{n!} \sum_{\alpha_i = \pm 1} \prod_i \alpha_i \;\; \det(\ldots)$$

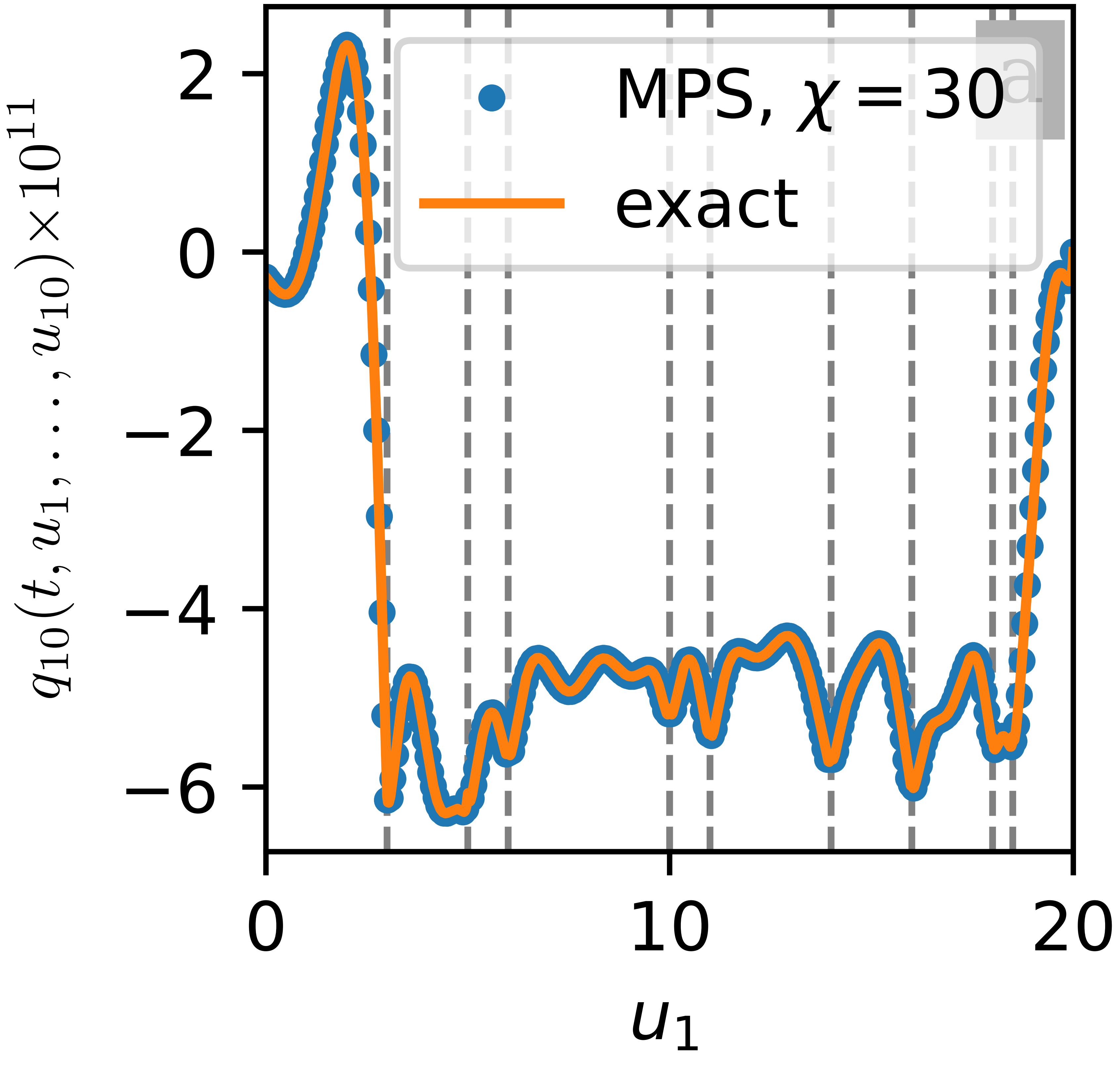
- q_n is ε-factorizable, in the *time differences v_i* (using a time-ordered domain in u_i)

$$v_1 = t - u_1$$
$$v_i = u_{i-1} - u_i \qquad \text{for } 2 \leq i \leq n.$$

$$\boxed{q_n(t, u_1, \ldots, u_n) \approx M_1(v_1) \ldots M_n(v_n)}$$

- Rank (bond dimension) χ
- Calculations for Q = charge on the quantum dot.

q_{10} vs its MPS interpolation



A non "standard" use of tensor networks

DMRG, PEPS, …

- MPS Ansatz for the many-body wavefunction ψ
- ψ is unknown
- Found by energy minimization.

TCI

- MPS compression of the (bare) n-body correlation functions $q_n(u_i)$.
- $q_n(u_i)$ is known
- Use the compressed form to integrate
- "Active" machine learning technique

Tensor Cross Interpolation

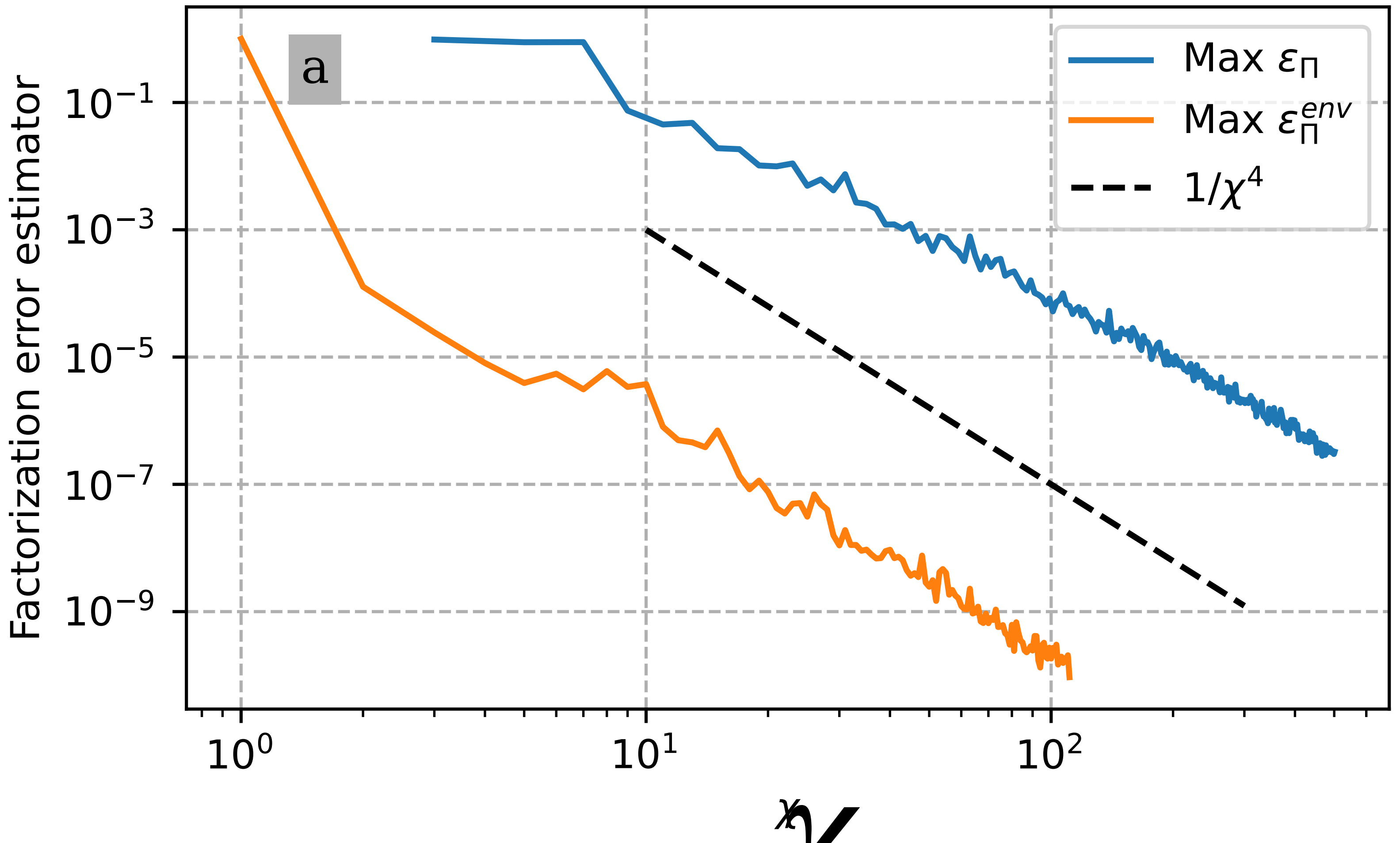
*I. **Oseledets and E. Tyrtyshnikov**, Linear Algebra and its Applications 432, 70 (2010).*
***I. V. Oseledets,** SIAM Journal on Scientific Computing 33, 2295 (2011).*
***D. V. Savostyanov,** Linear Algebra and its Applications 458, 217 (2014)*

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

Tensor Cross Interpolation (TCI)

- Given a n-dimensional tensor $A(u_1, u_2, \ldots, u_n)$ [u_i are discrete indices with d values]
- It builds a MPS approximation A_χ^{TCI} of A of rank χ, progressively increasing χ
- From the evaluation of A on N points with $N \sim nd\chi^2 \ll d^n$
- With an error estimator $\epsilon(\chi)$, decreasing with χ when the algorithm is successful

$\epsilon(\chi)$



χ

Error estimators

$q_{10},\ \epsilon_d = 0$

Low rank decomposition of a matrix

- A is a M x N matrix of low rank.
- Singular Value Decomposition (SVD).
  - Need the full matrix
- Cross Interpolation (CI)
  - Pivots : subset of rows/columns $: I = \{i_1, i_2, \ldots, i_\chi\}, \quad J = \{j_1, j_2, \ldots, j_\chi\}$

Slices

$$A = A(\mathbb{I}, \mathbb{J}) \approx A(\mathbb{I}, J)A(I, J)^{-1}A(I, \mathbb{J})$$

$\mathbb{I} = \{1, 2, \ldots, M\}$
$\mathbb{J} = \{1, 2, \ldots, N\}$

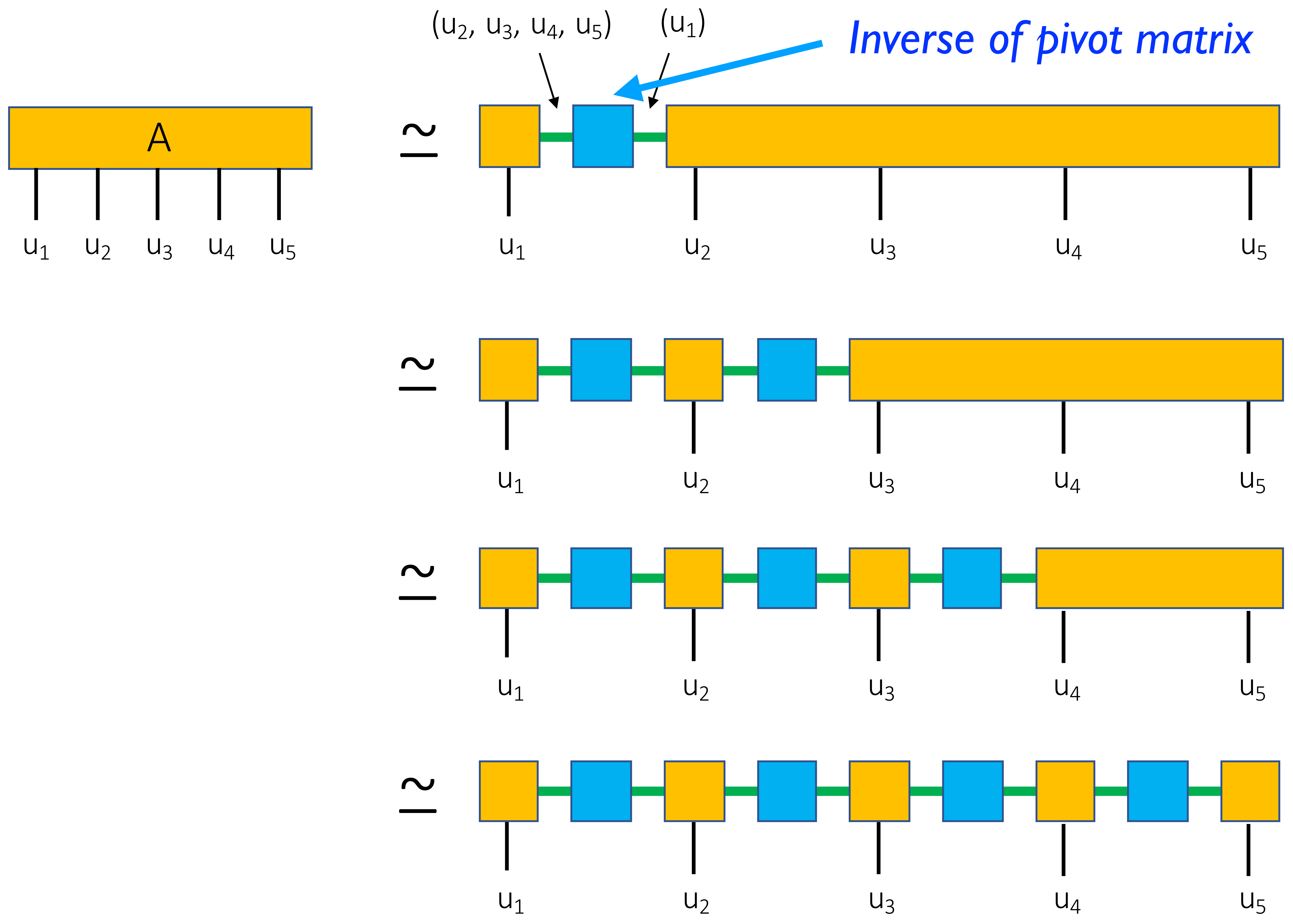
Pivots
Submatrix of A of size $\chi \times \chi$

Properties

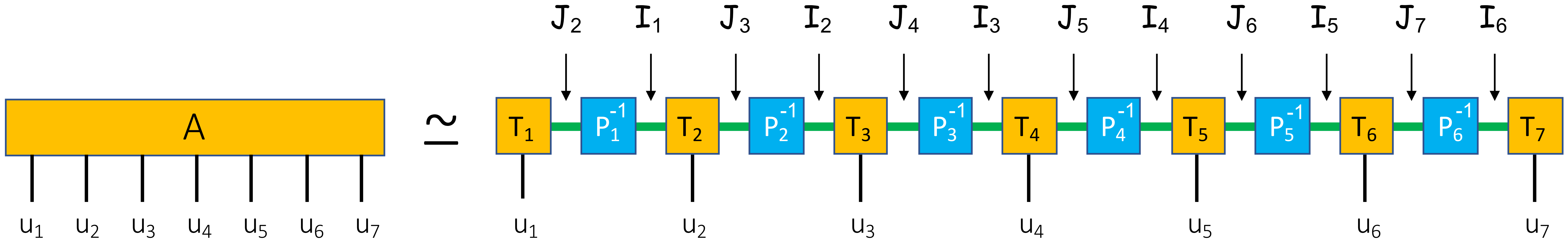
1. Interpolation : exact on the pivots indices
2. If A is of rank χ, it is exact

Tensor case

- $n-$dimensional tensor $A(u_1, u_2, \ldots, u_n)$ [u_i are discrete or continuous indices]
- Naive approach: repeated application of the matrix case (grouping indices)



Tensor Cross Interpolation (TCI)



$\equiv A^{TCI}(u_1, \ldots, u_n)$

- Pivots: set of multi-indices $(1 \leq \alpha \leq n)$

$$I_\alpha = \{i_1, \ldots, i_\chi\} \qquad J_{\alpha+1} = \{j_1, \ldots, j_\chi\}$$
$$i = (u_1, \ldots, u_\alpha) \qquad j = (u_{\alpha+1}, \ldots, u_n)$$

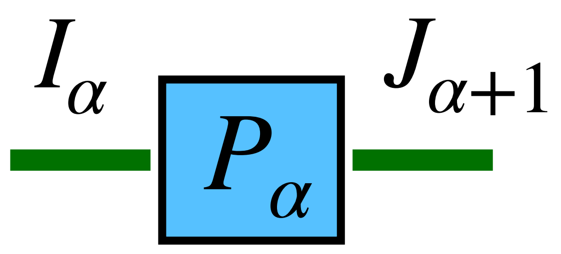
$$i \oplus j \equiv (u_1, \ldots, u_n)$$
$$I_\alpha \oplus J_{\alpha+1} \equiv \{i \oplus j \,|\, i \in I_\alpha, j \in J_{\alpha+1}\}$$

- Set of d values of u_α : $\mathcal{U}_\alpha \equiv \{(u_\alpha)\}$

- T, P are subarrays of A

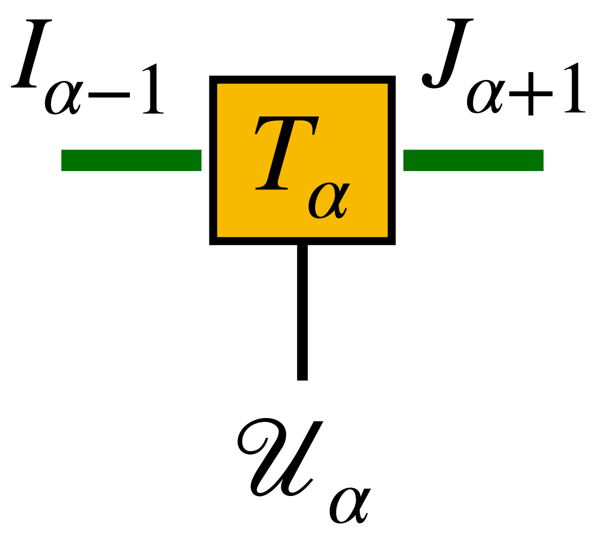
- *Pivots matrices*

$$P_\alpha \equiv A(I_\alpha \oplus J_{\alpha+1})$$



- *1d slices*

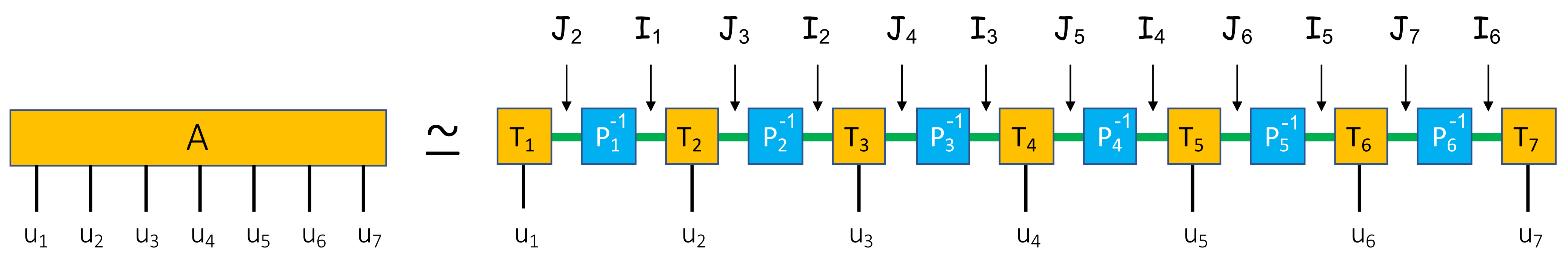
$$T_\alpha \equiv A(I_{\alpha-1} \oplus \mathcal{U}_\alpha \oplus J_{\alpha+1})$$



- TCI is exact on 1d slices

$$T_\alpha = A^{TCI}(I_{\alpha-1} \oplus \mathcal{U}_\alpha \oplus J_{\alpha+1})$$

TCI algorithm



- Add new pivots to reduce the interpolation error <u>on 2d slices</u>

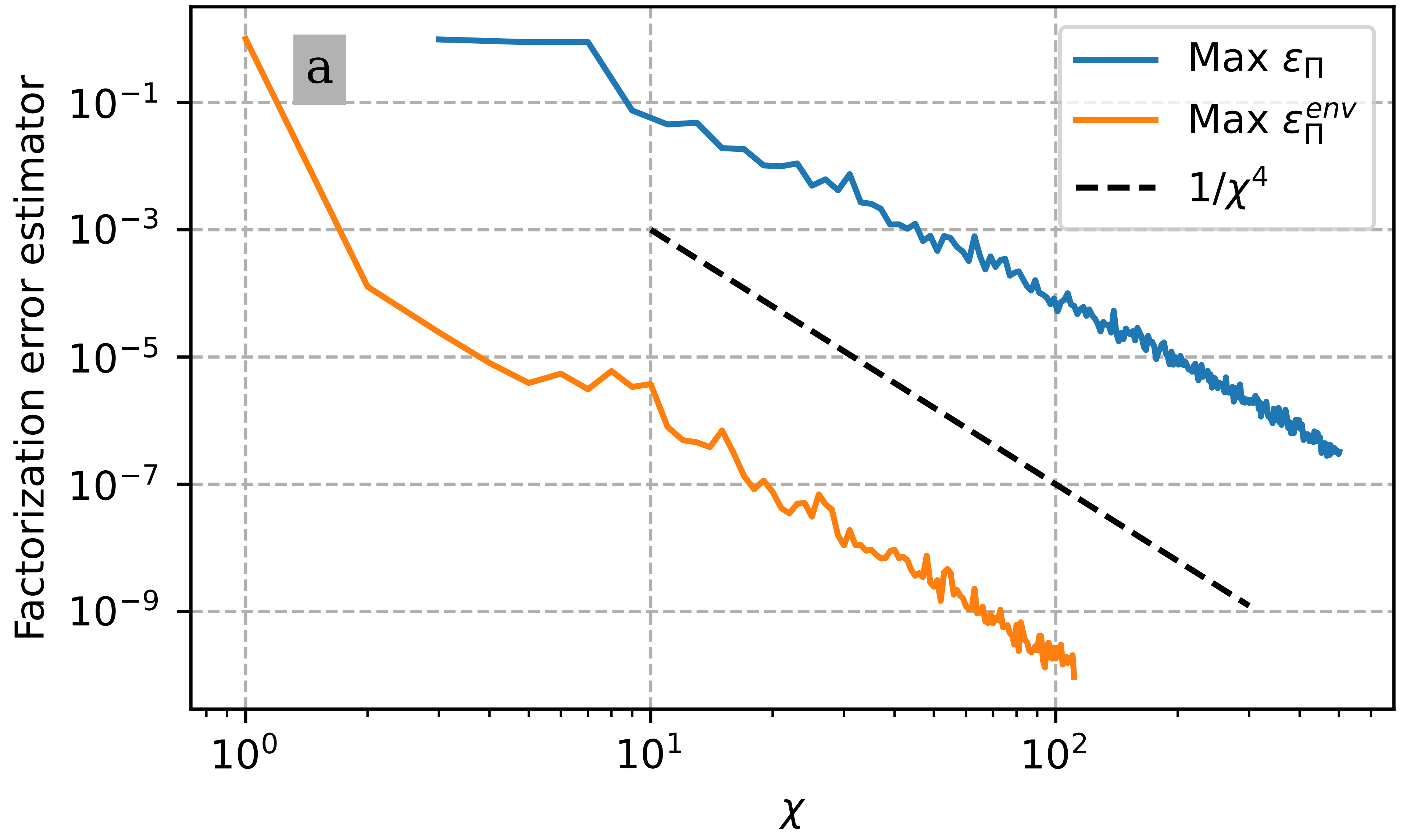
$$\epsilon_\Pi(i, u_\alpha, u_{\alpha+1}, j) = |A - A^{TCI}|(i, u_\alpha, u_{\alpha+1}, j),\ \text{for } i \in I_{\alpha-1}, j \in J_{\alpha+2}$$

Add pivots at the point where error is maximal
Sweep over the tensor, for all α

- Factorization error estimator

$$\epsilon(\chi) = \max_{\alpha} \max_{i,j,u_\alpha,u_{\alpha+1}} \epsilon_\Pi(i, u_\alpha, u_{\alpha+1}, j)$$

Error estimators
q_{10}, $\epsilon_d = 0$

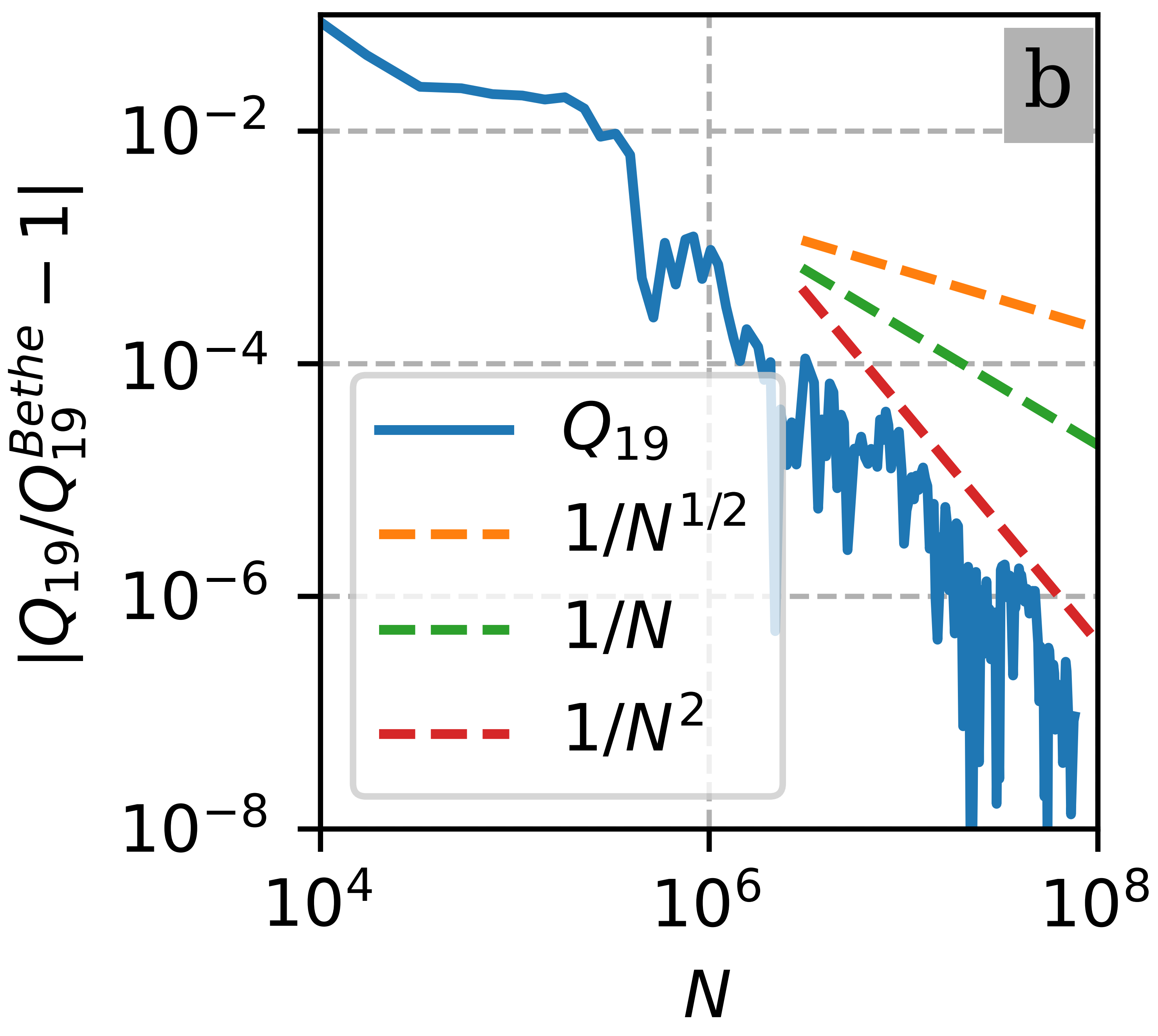


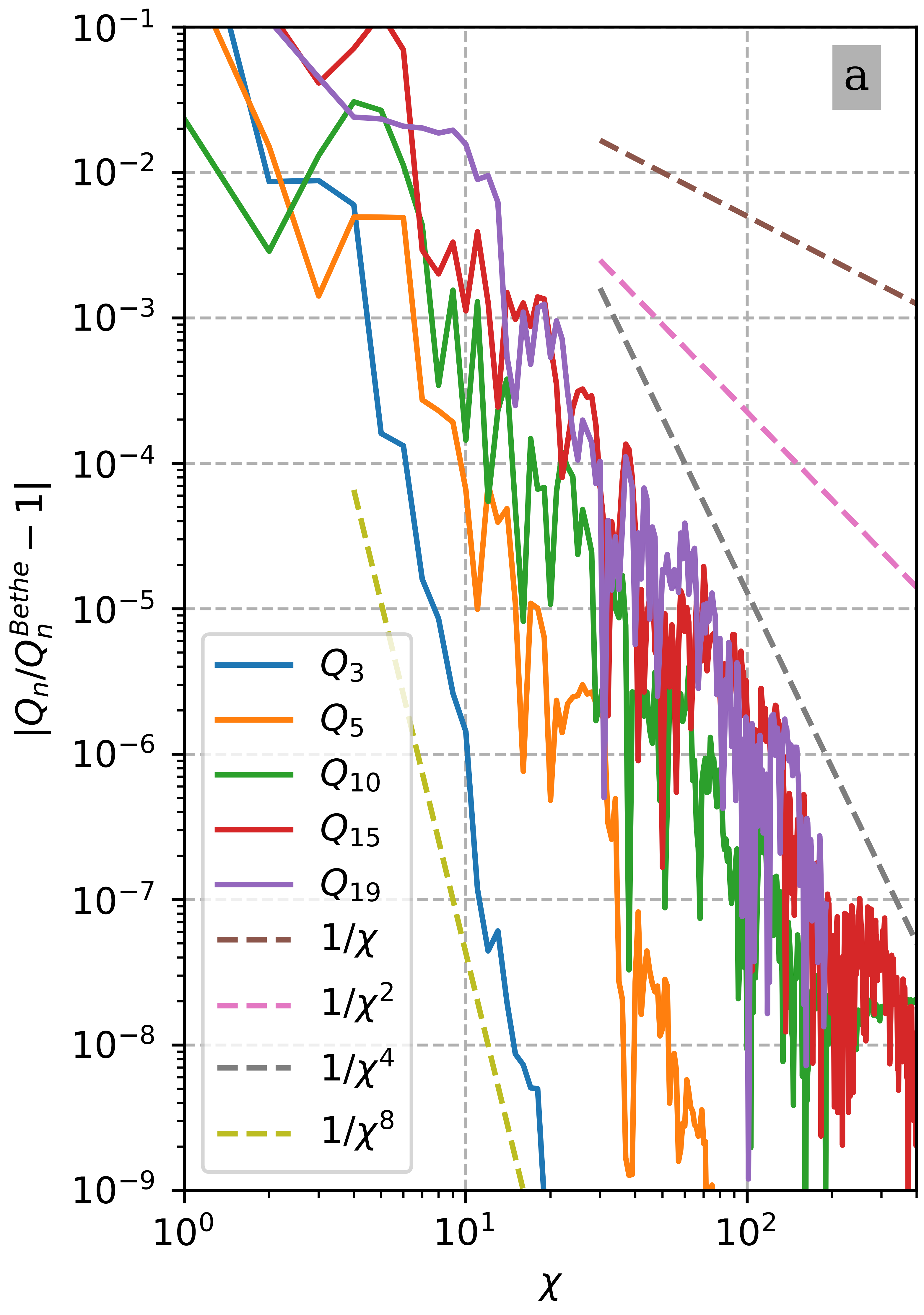
Tensor Train Diagrammatics

Benchmarks for a quantum dot in equilibrium

Tensor Train Diagrammatics

- Factorize q_n with TCI and integrate
- High precision (9 digits) benchmark vs Bethe Ansatz.
- N (number of evaluations of q_n) : $N \sim \chi^2$
- Convergence rate : error $\sim 1/N^2$

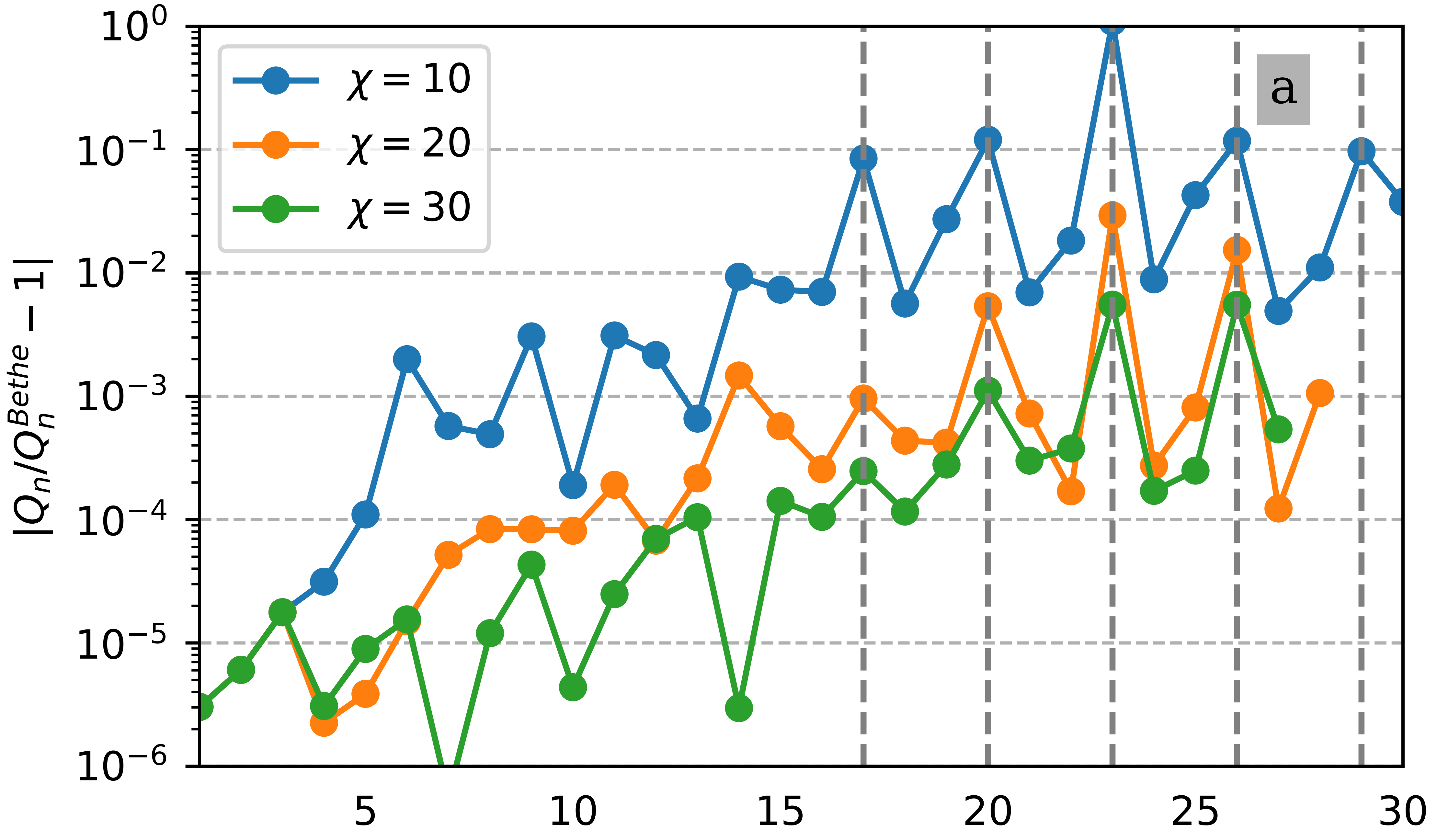




χ does not grow with dimension n

- Compute Q_n up to n = 30

$$|Q_n/Q_n^{Bethe} - 1|$$

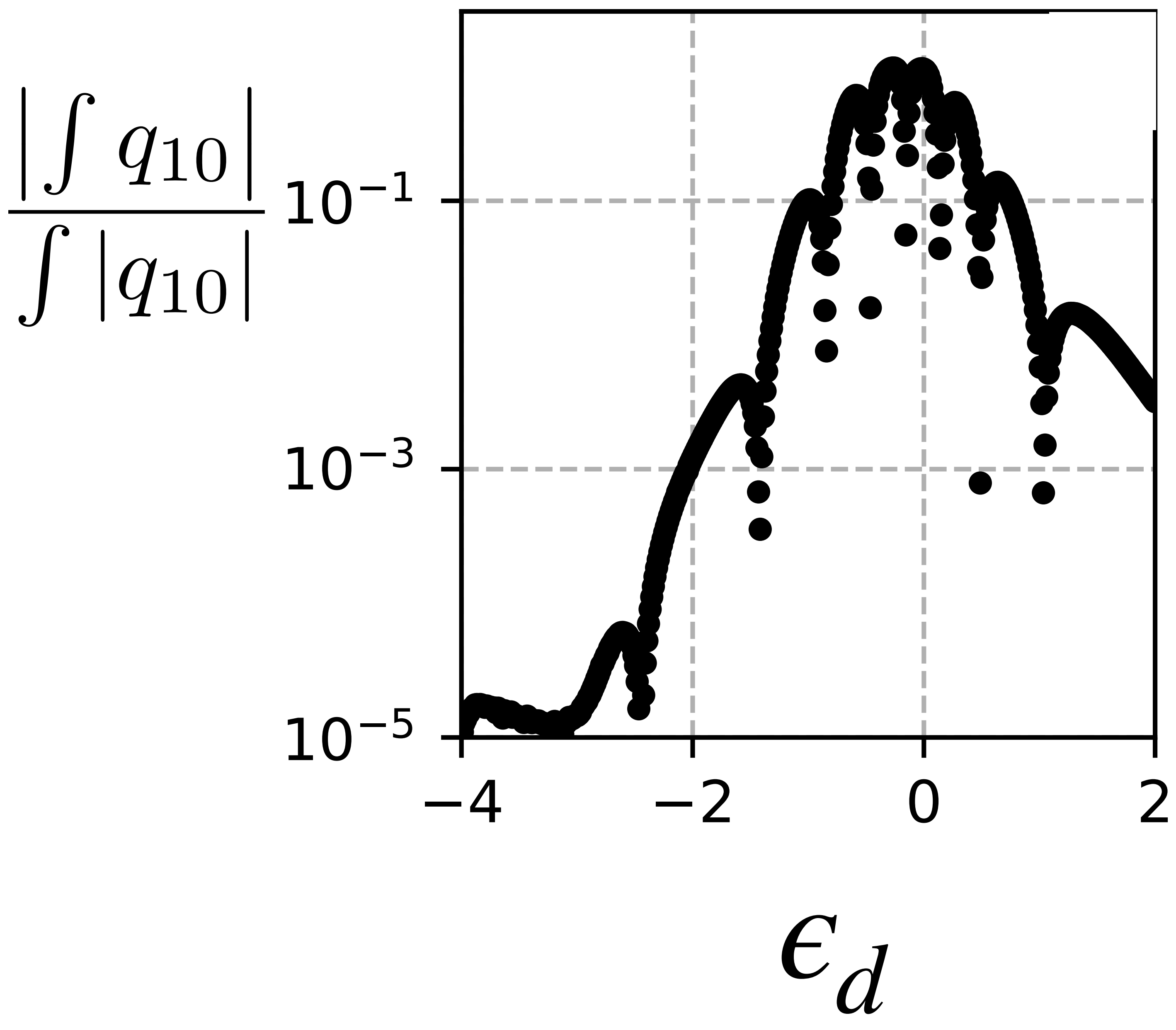


n

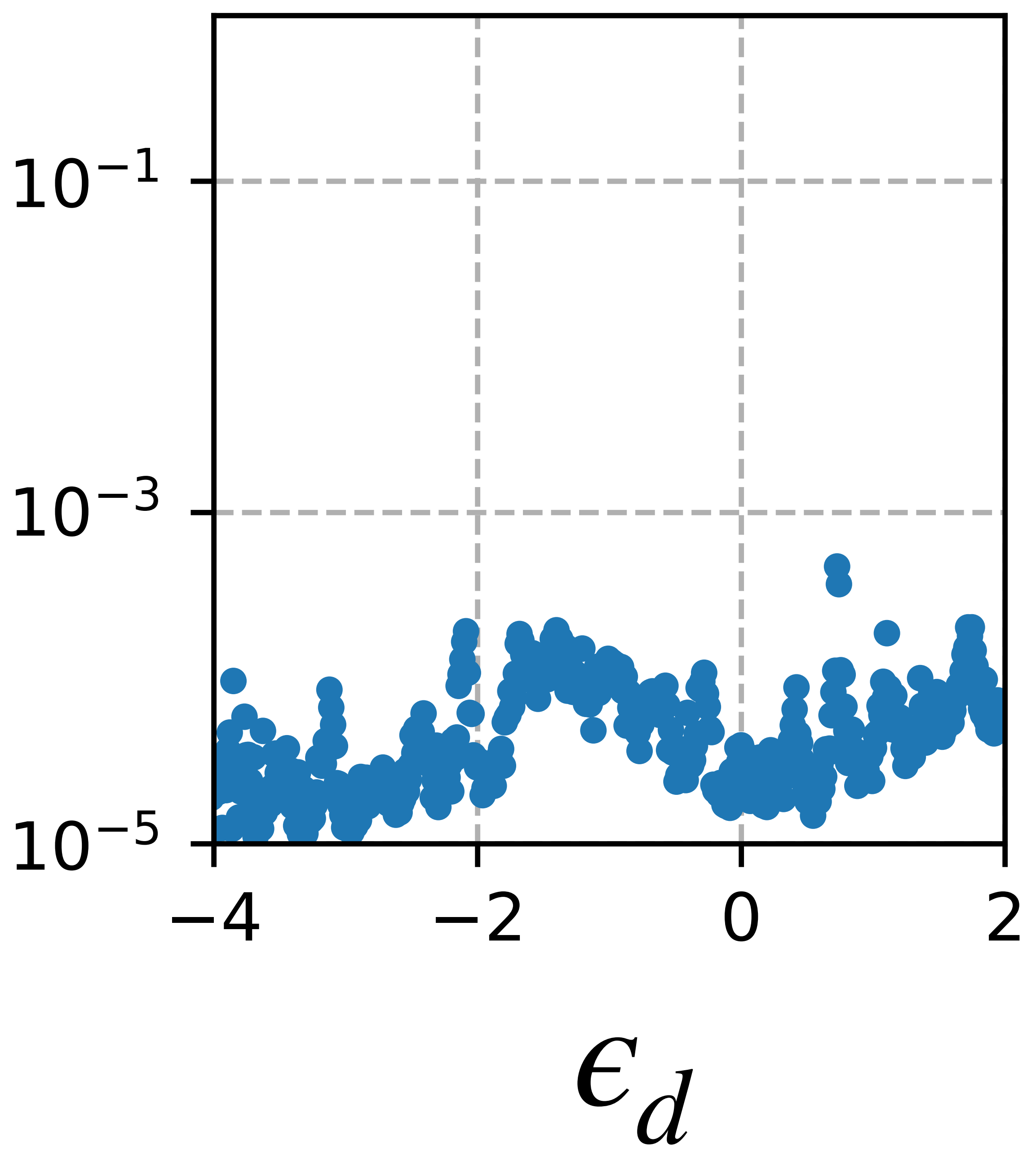
Factorize the sign problem

- The factorization is insensitive to the average sign of the function.
- Reduced to a 1d oscillating integral.
- Example: vary dot energy level ϵ_d (induces oscillating terms $e^{i\epsilon_d t}$)

Average sign of the Q_{10} integral



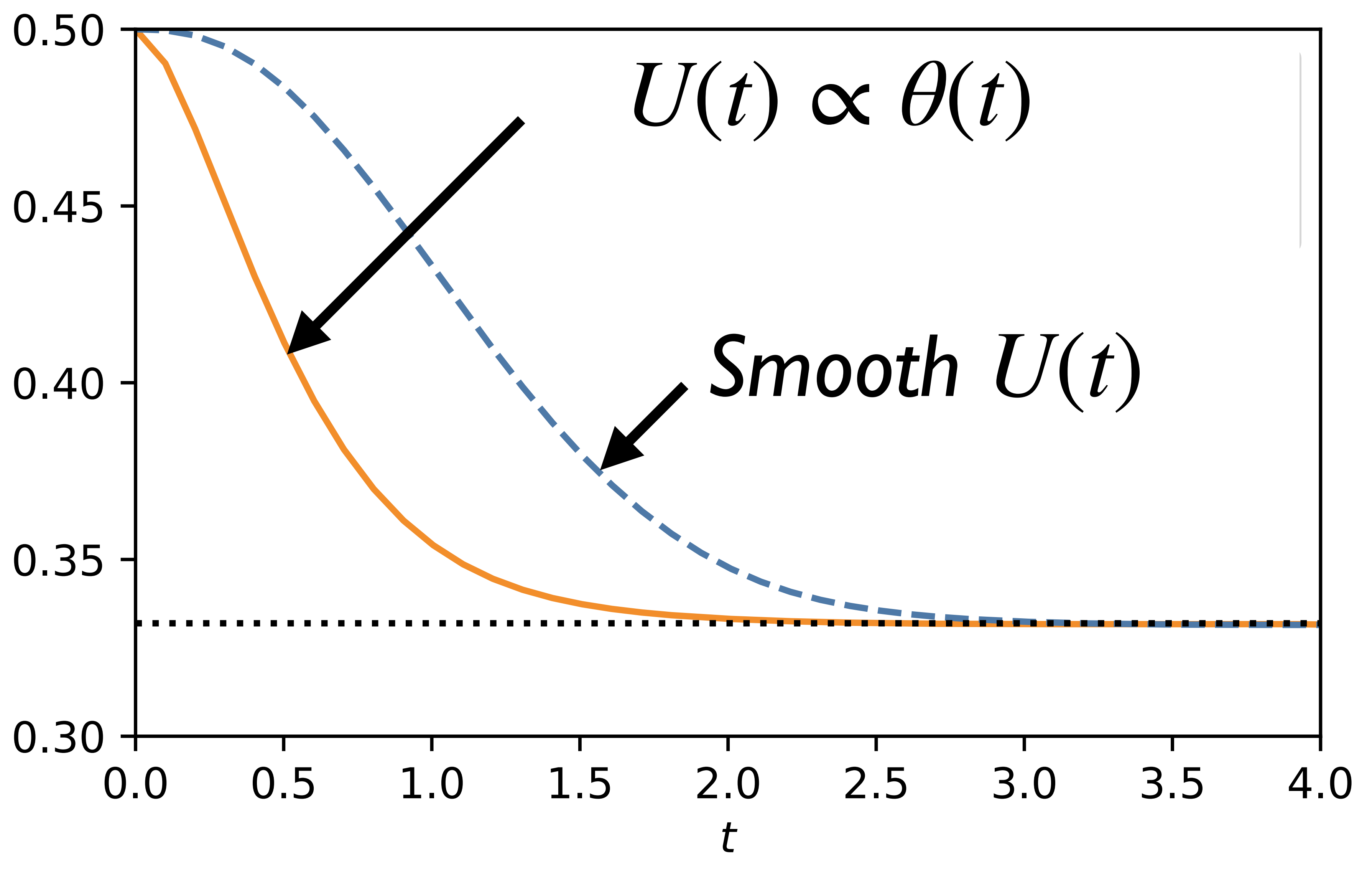
Factorization error of q_{10} for fixed bond dimension χ



Full time dynamics from a single factorization

$$Q_n(t) = \int_{t_0}^{\infty} du_1 \dots du_n \ \ q_n(t, u_1, \dots, u_n)$$

- Since we factorize the integrand q_n, we obtain as post-processing
  - The full time dependency : $Q_n(t)$ vs t (restrict the integration domain)
  - The effect of any time dependent coupling constant (multiply q_n in the integral)



Charge of quantum dot $Q(t)$ for $U = 2$

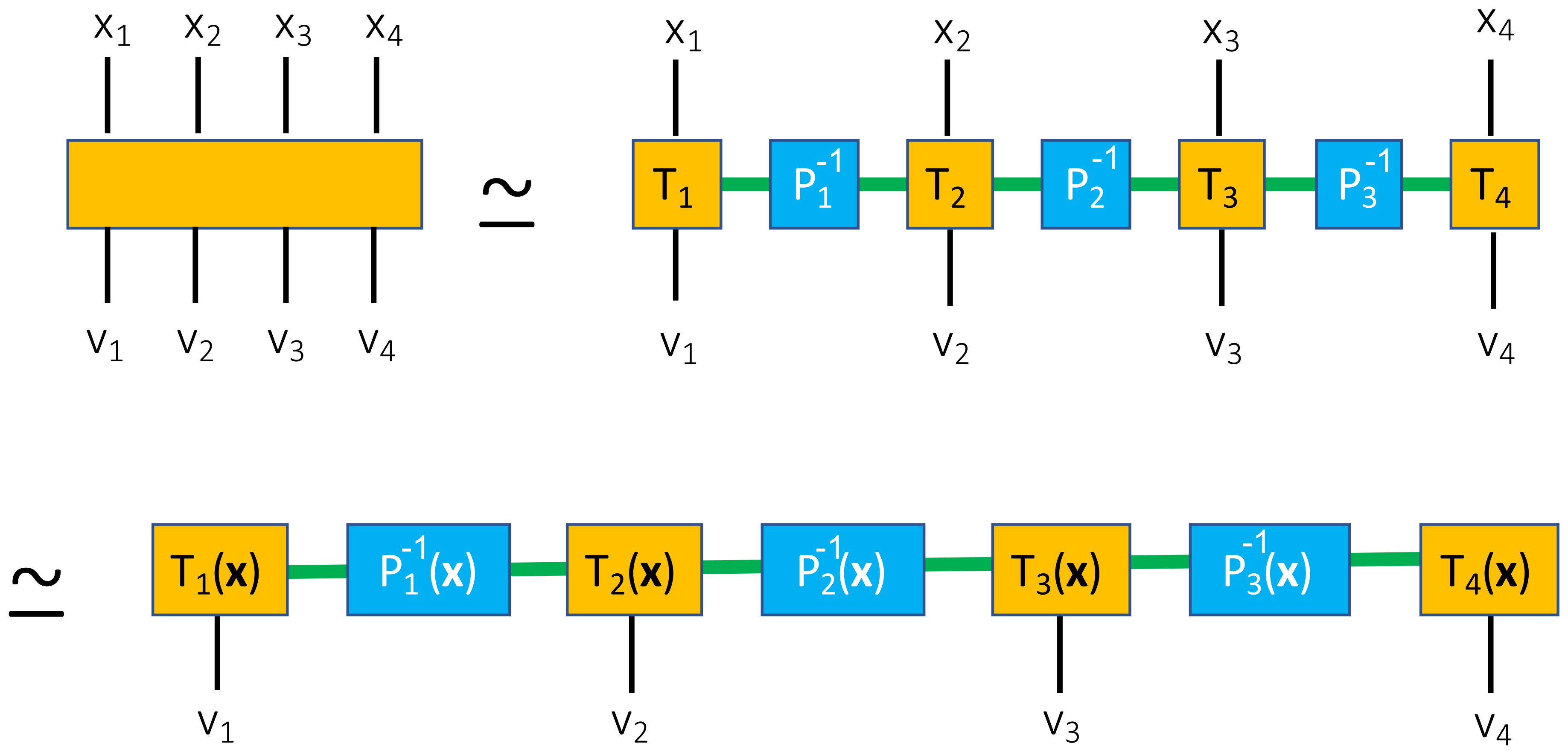
Towards lattice models …

Multiple quantum dots

- Integrate on space and time

$$Q_n(t) = \int_{t_0}^{\infty} du_1 \ldots du_n \sum_{x_1,\ldots,x_n} q_n(t, u_1, x_1, \ldots, u_n, x_n)$$

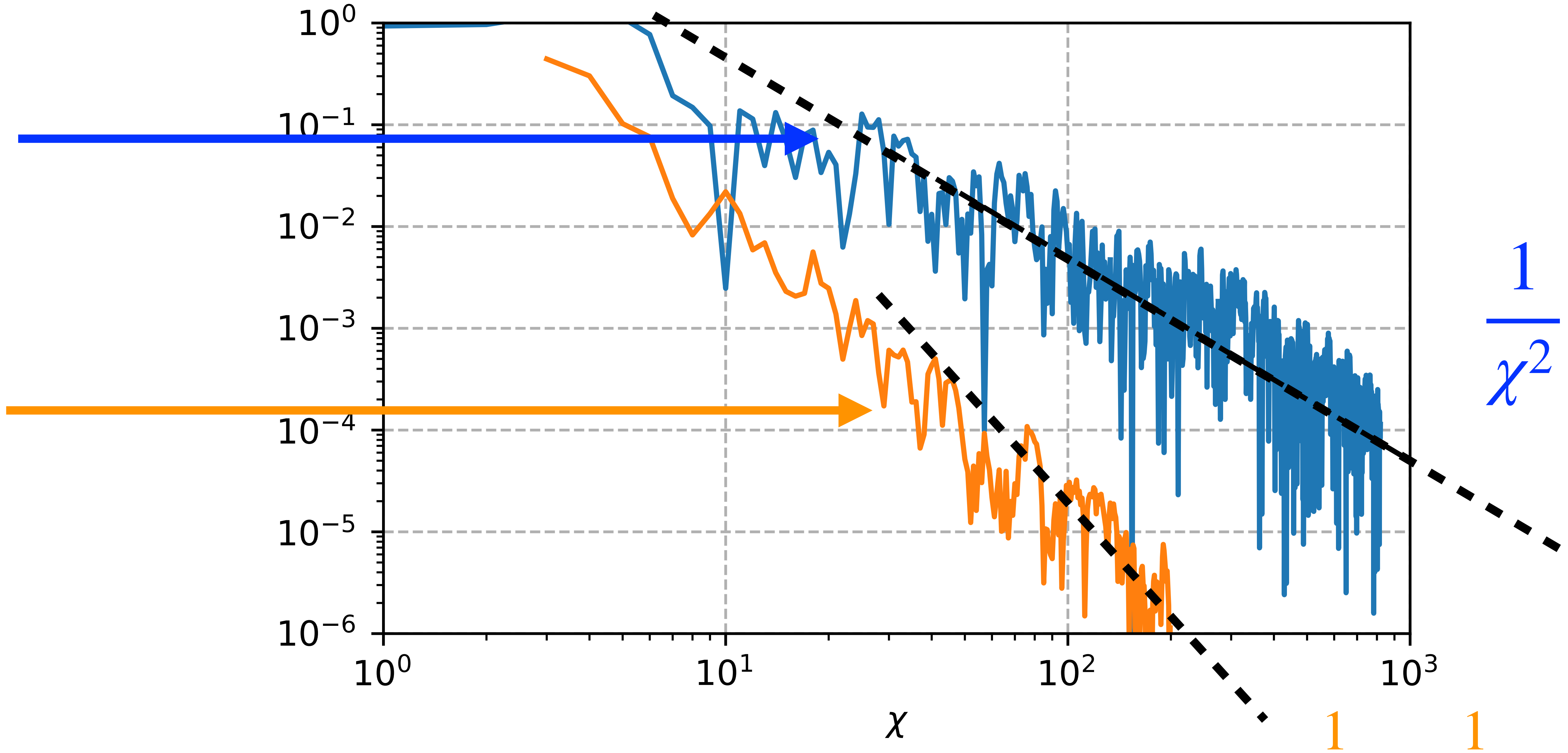
- Form of the tensor network ? Beyond MPS ?



Brute force sum over x

$$\left| \frac{Q_{10}(\chi)}{Q_{10}^{ref}(\chi)} - 1 \right|$$

Double dot



$$\frac{1}{\chi^2} \sim \frac{1}{N}$$

$$\frac{1}{\chi^4} \sim \frac{1}{N^2}$$

Tensor Cross Interpolation
Another way of using tensors

- Various potential applications
  - Replace QMC in various diagrammatics techniques, e.g real or imaginary time, inchworms *G. Cohen et al. PRL (2015), E. Eidelstein et al. PRL (2020).*
  - Find "Quantics" decomposition of functions. *arXiv:2303.11819*
  - …

Revisiting CTQMC in imaginary time

- Quantum impurity model

$$S_{eff} = \int d\tau \sum_a c_a^\dagger(\tau)\left(\partial_\tau - \mu\right)c_a(\tau) + H_{atomic}(c^\dagger, c) + \int d\tau d\tau' c_a^\dagger(\tau)\Delta_{ab}(\tau - \tau')c_b(\tau')$$

- Expansion of the partition function Z in power of Δ at all orders

$$Z = \sum_{n\geq 0} \int_0^\beta \prod_{i=1}^n d\tau_i d\tau_i' \quad z_n(\tau_1, \ldots, \tau_n)$$

- Continuous time QMC (CT-HYB algorithm) computes the series and the integrals.

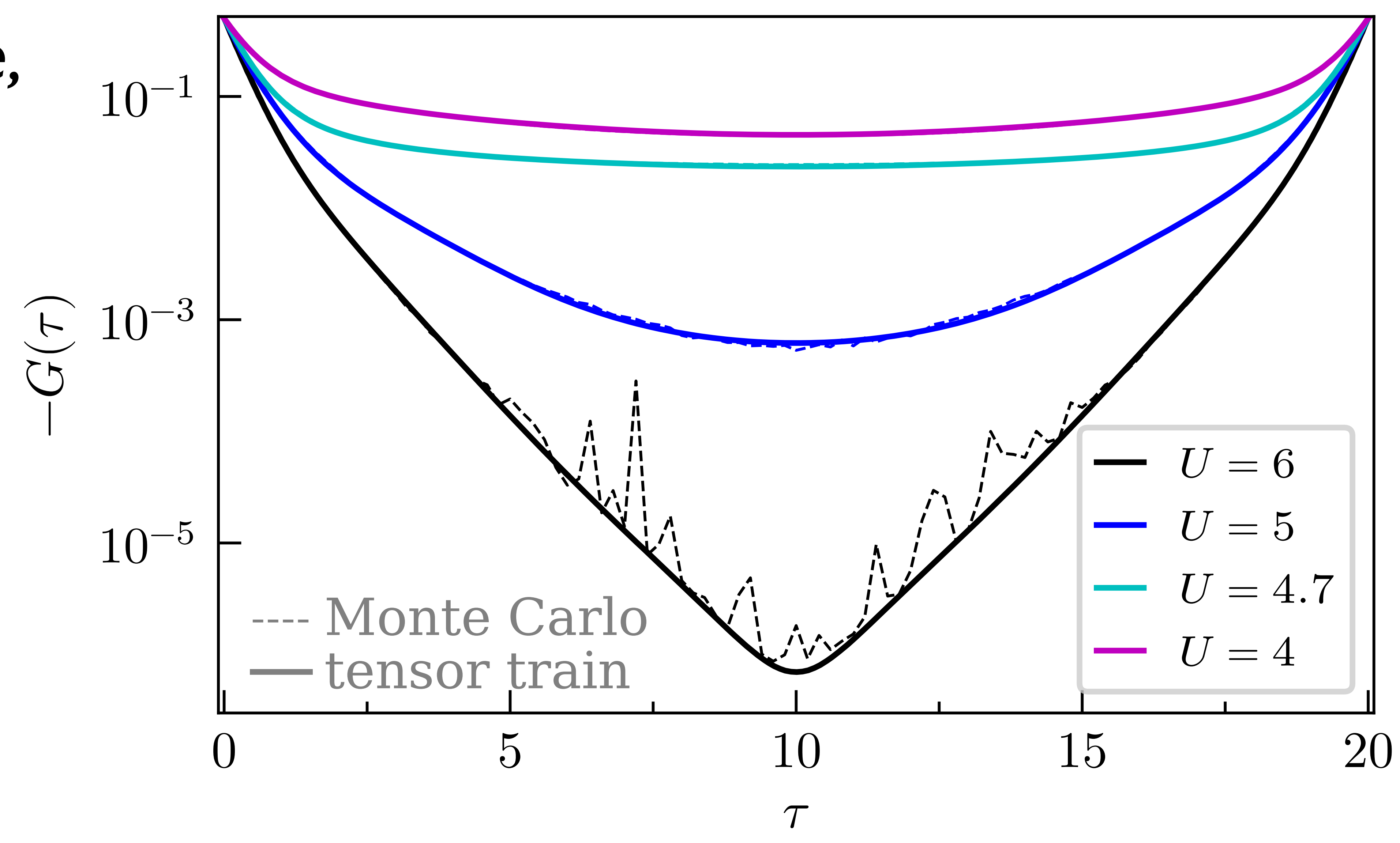
P. Werner et al. PRL. 97, 076405 (2006)

Can we use TCI instead of QMC ?

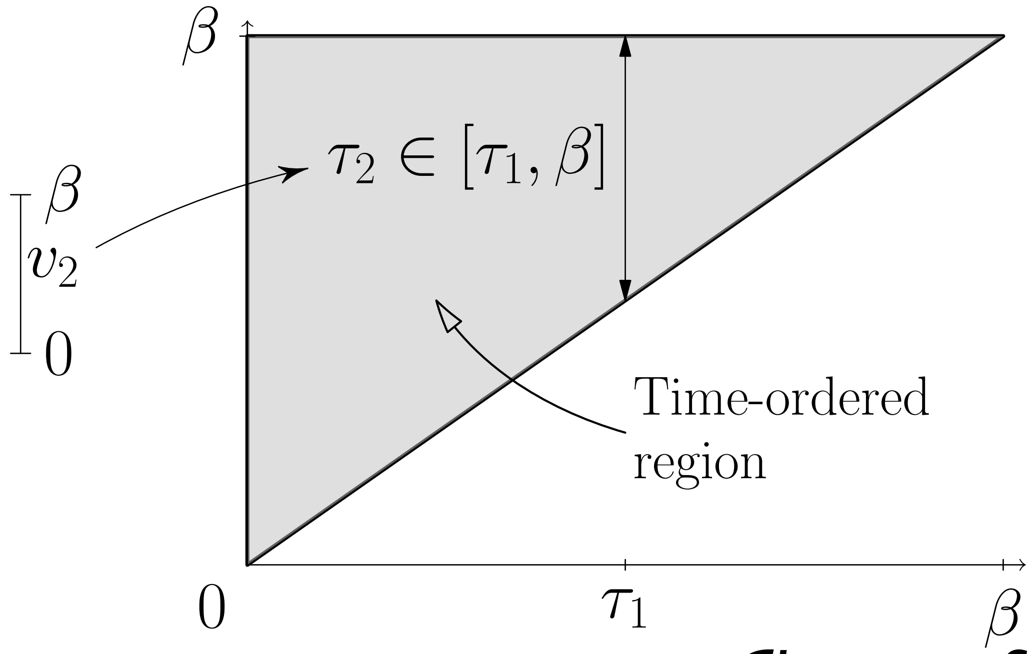
TCI-Hybridization expansion

- Use TCI to compute the integrals instead of MC

DMFT solution, Bethe lattice, for various U vs CTQMC
$\beta t = 20$



A. Erpenbeck, W.-T. Lin, *T. Blommel, L. Zhang, S. Iskakov, L. Bernheimer, Y. Núñez-Fernández, G. Cohen, O. Parcollet, X. Waintal, E. Gull*
arXiv:2303.11199 (To appear in Phys. Rev. B)



Change of variables $\tau_i \to v_i$

- Precise computation of Z, Free energy
- One band model, moderate temperature ($\beta t \sim 40$)
- Next step: multiorbital case, in regimes where QMC has a severe sign problem.

Conclusion

- Out of equilibrium solutions using perturbative series
  - Even at long time, even in strong coupling regimes.
- Tensor train diagrammatics
  - Replace Monte Carlo with Tensor Cross Interpolation (TCI).
  - Insensitive to the sign problem.
  - TCI : A robust technique with multiple potential applications.

Thank you for your attention!