Computational Quantum Many-Body Physics:
A few highlights

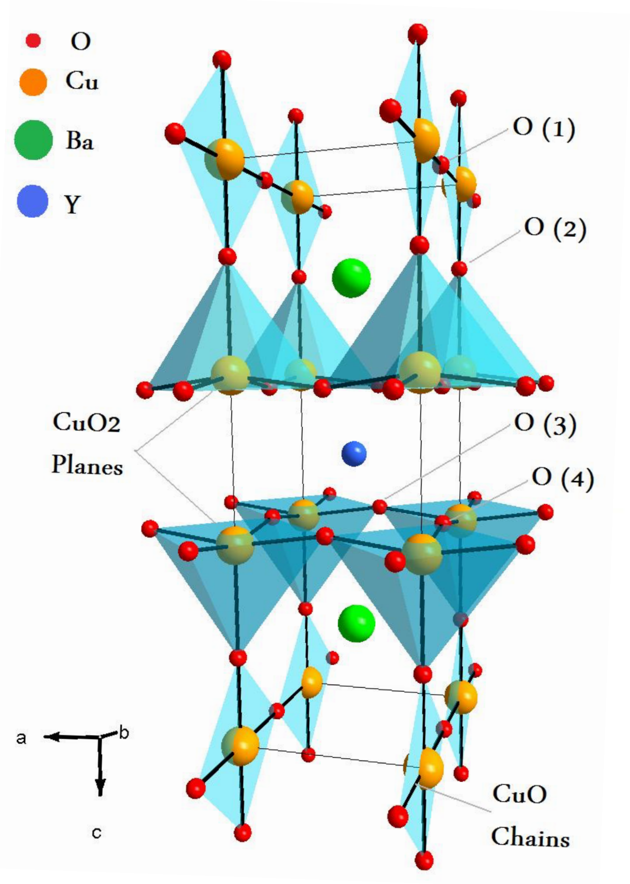
Olivier Parcollet

Center for Computational Quantum Physics
Flatiron Institute, Simons Foundation,
New York
&
IPhT, Saclay

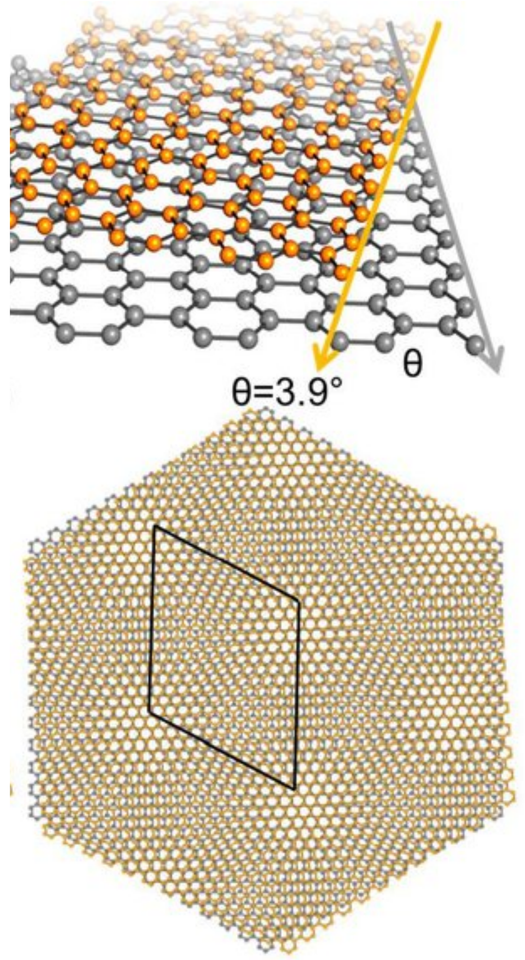
The quantum many-body problem

- Many interacting quantum particles
- At low temperature. Collective effects.
- “More is different” *Anderson, 73*

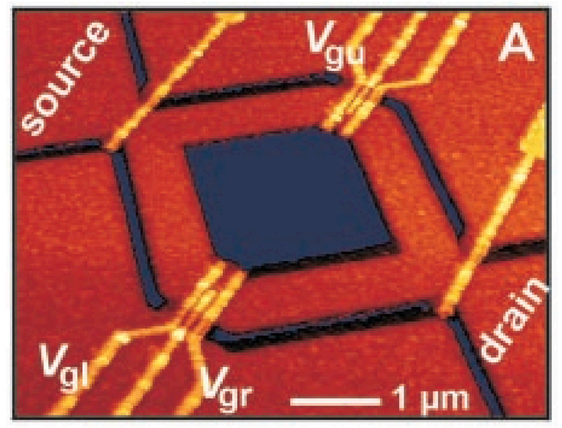
- Examples:
    - Electrons in solids.
    - Nano-electronics
    - Quantum Chemistry.
    - Quantum optics. Ultra-cold atoms
    - Nuclear physics. QCD.



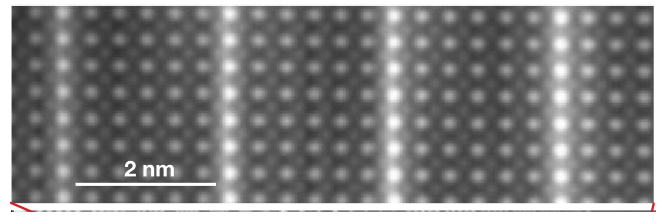
High Temperature superconductors



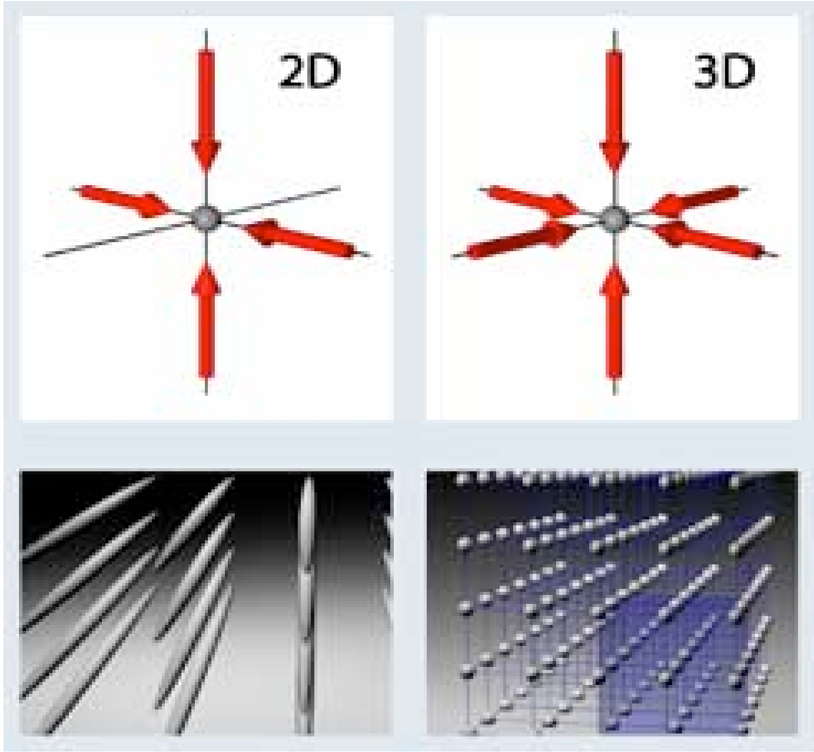
Moiré systems



Quantum dot



Interfaces



Ultra-cold atoms in optical lattices

Quantum Many-Body problem

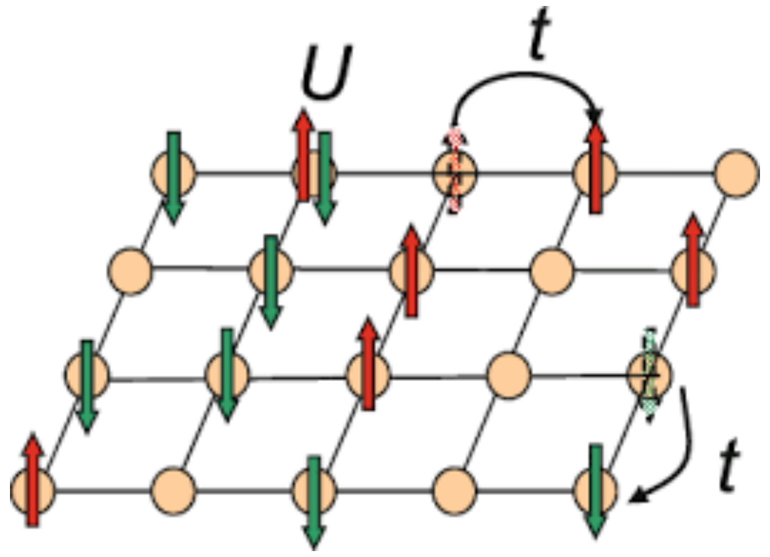
- A central topic at IPhT, with many contributions
  e.g. *C. De Dominicis, C. Bloch, J.P. Blaizot, H. Orland, G. Ripka, R. Balian, …*
- Very close to:
  - Quantum field theory.
  - Condensed matter theory.

Computational Quantum Many body physics

Develop concepts/methods/algorithms to solve quantum many body systems

Simplified Models

- e.g. Hubbard model

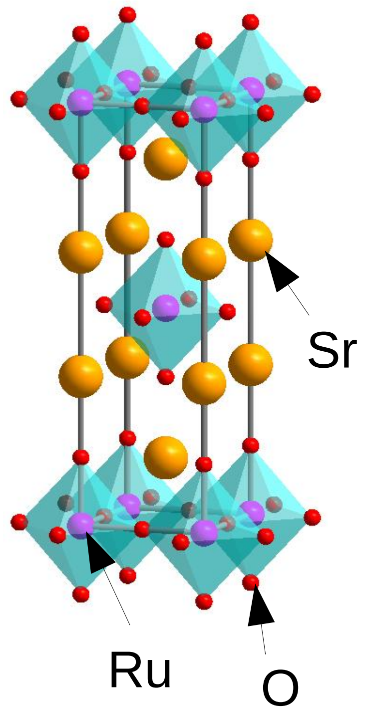


$$H = -\sum_{\langle ij\rangle,\sigma=\uparrow,\downarrow} t\; c^\dagger_{i\sigma} c_{j\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow}$$

Nearest neighbours

Ab initio / realistic

- From first principles



$$H = \sum_{i=1}^{N} -\frac{\hbar^2}{2m}\nabla^2_{x_i} + V_{crystal}(x_i) + \sum_{i<j} \frac{e^2}{x_i - x_j}$$

Material design

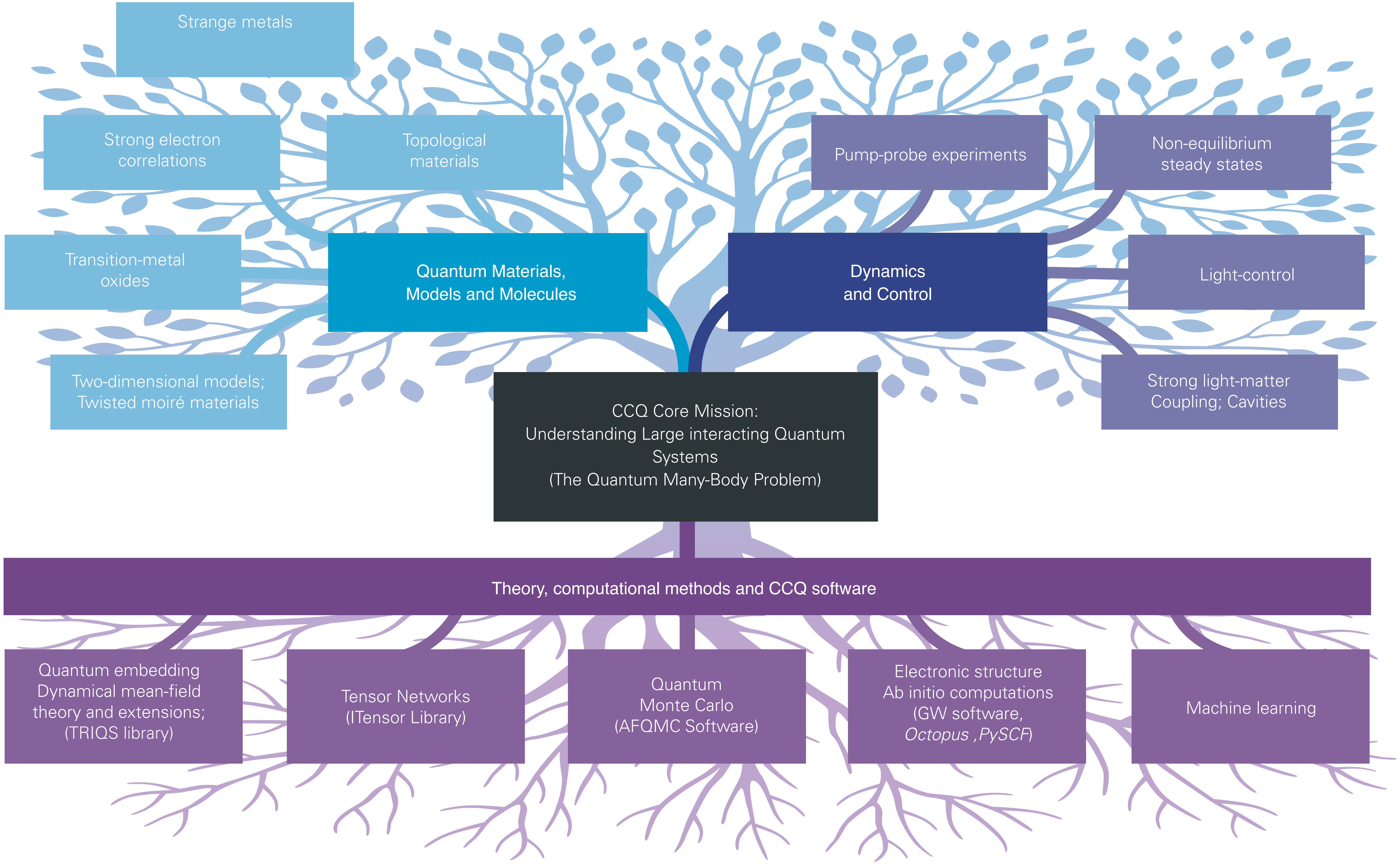
The Flatiron Institute / Simons Foundation

- Research institute of the Simons Foundation.
- 5 Centers.
  - Computational Astrophysics (CCA)
  - Computational Biology (CCB)
  - Computational Mathematics (CCM)
  - Computational Neurosciences (CCN)
  - Computational Quantum Physics (CCQ)
    $\sim$ 15 faculty, 25 postdocs; students, visitors.
    Since fall 2017.

Mission: "to develop the concepts, theories, algorithms and codes needed to solve the quantum many-body problem and use the solutions to predict the behavior of materials and molecules of scientific and technological interest."

Junior position open between CCQ and IPhT ! (Deadline Nov 15th)

The CCQ Research Ecosystem



Strange metals

Strong electron correlations

Topological materials

Transition-metal oxides

Two-dimensional models; Twisted moiré materials

Quantum Materials, Models and Molecules

Dynamics and Control

Pump-probe experiments

Non-equilibrium steady states

Light-control

Strong light-matter Coupling; Cavities

CCQ Core Mission:
Understanding Large interacting Quantum Systems
(The Quantum Many-Body Problem)

Theory, computational methods and CCQ software

Quantum embedding Dynamical mean-field theory and extensions; (TRIQS library)

Tensor Networks (ITensor Library)

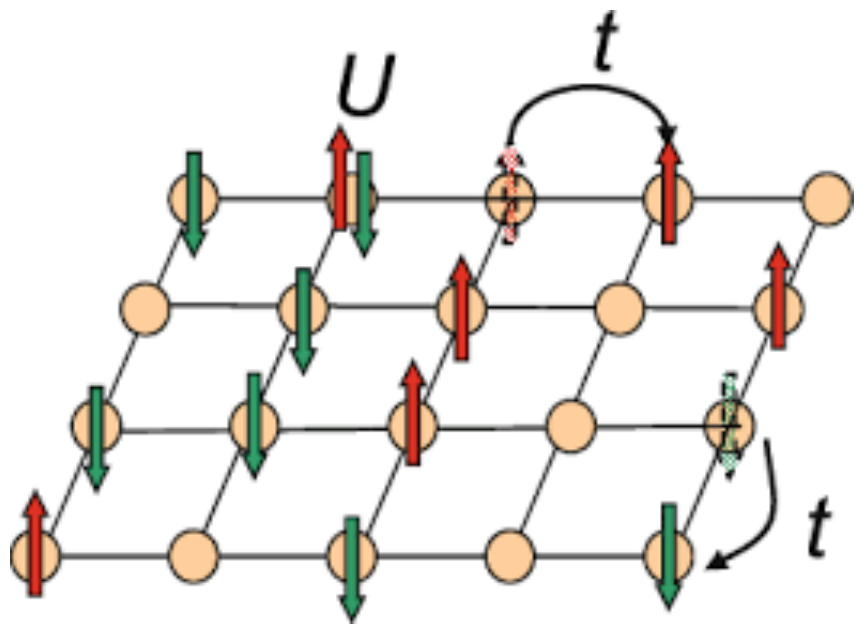
Quantum Monte Carlo (AFQMC Software)

Electronic structure Ab initio computations (GW software, *Octopus* ,*PySCF*)

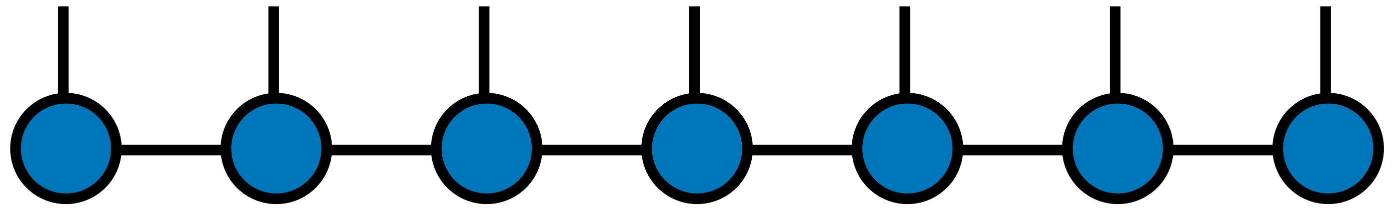
Machine learning

Parsimonious representations

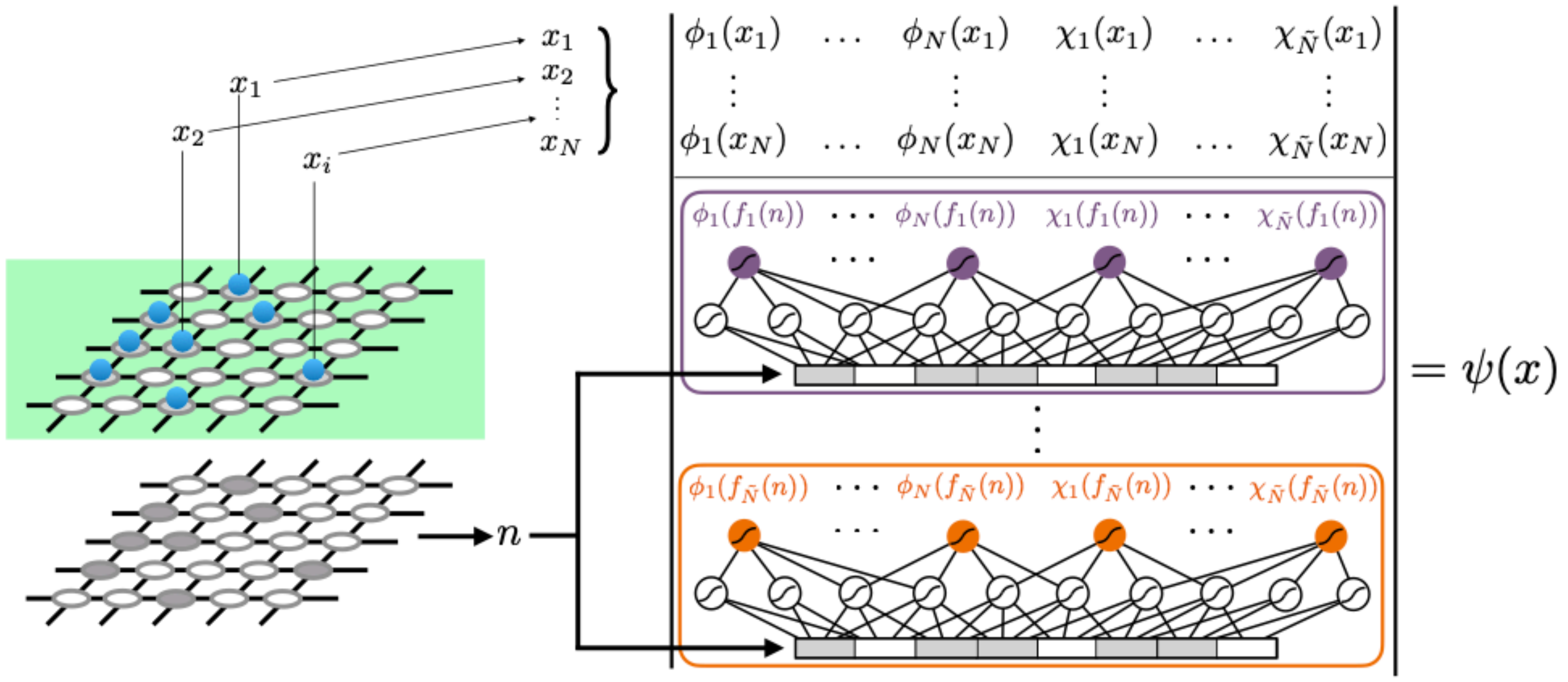
- Compressed representation of wavefunctions $\psi(x_1, \ldots, x_N)$/ correlations functions
- Overcome the exponential scaling of the N-body problem.



Tensor Network



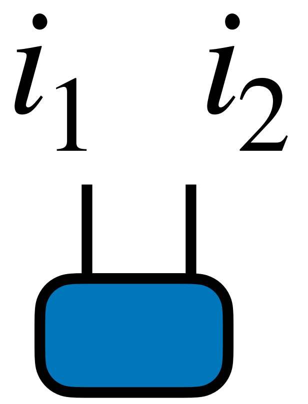
Machine learning



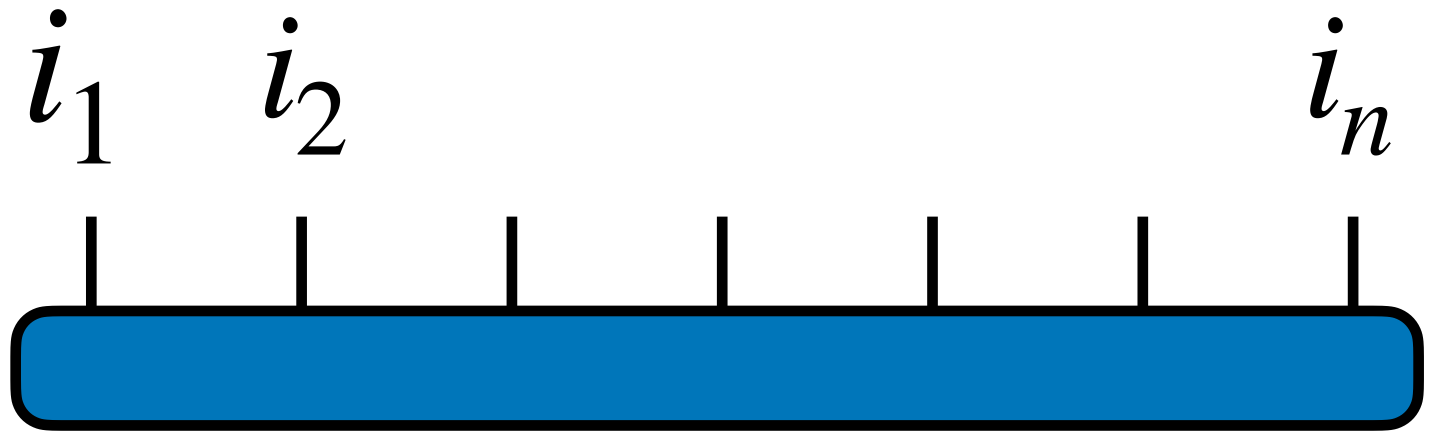
G. Carleo, M. Troyer Science (2017),
J Robledo-Moreno et al. PNAS (2022)

Tensors

- A n-dimensional array $T_{i_1 i_2 \ldots i_n}$ with the indices $i_k \in \{1,\ldots,d\}$
- Pictorial representation.
  Legs = indices.
  Contraction = connecting lines.



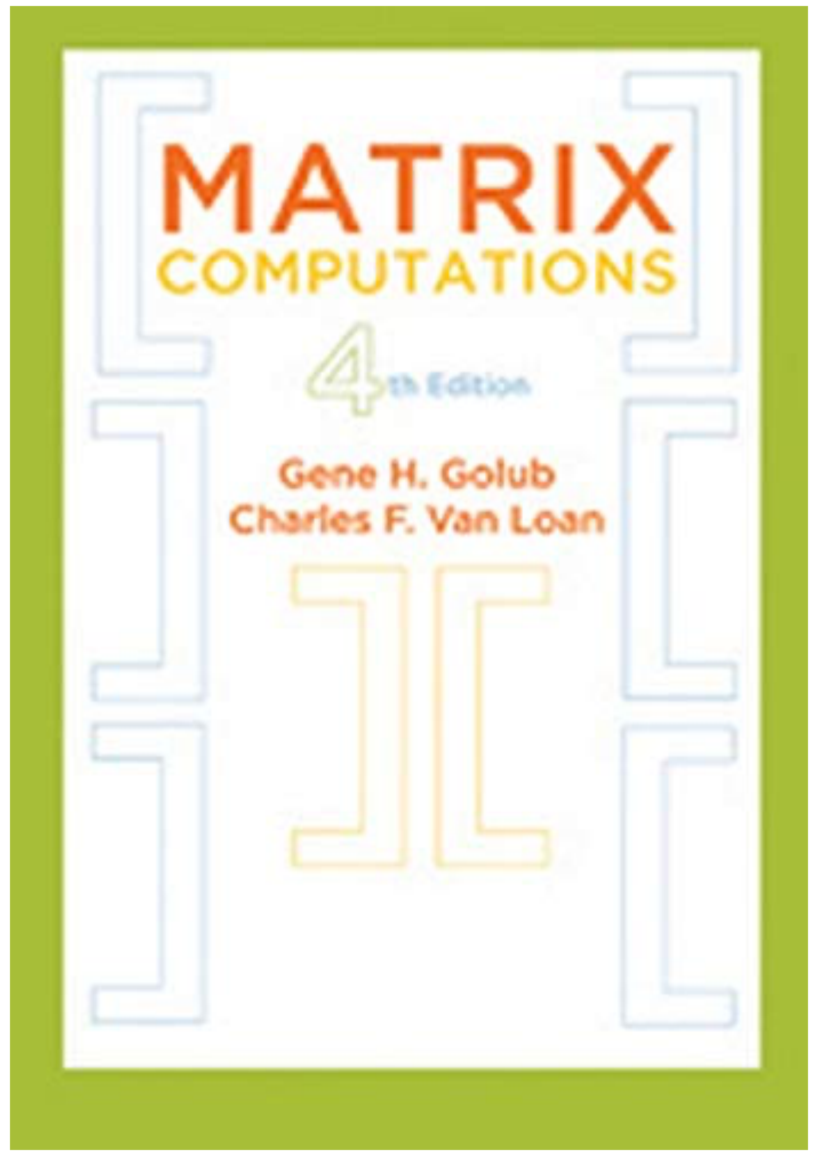
$A_{i_1 i_2}$



$T_{i_1 i_2 \ldots i_n}$

Low rank decomposition of tensors ?

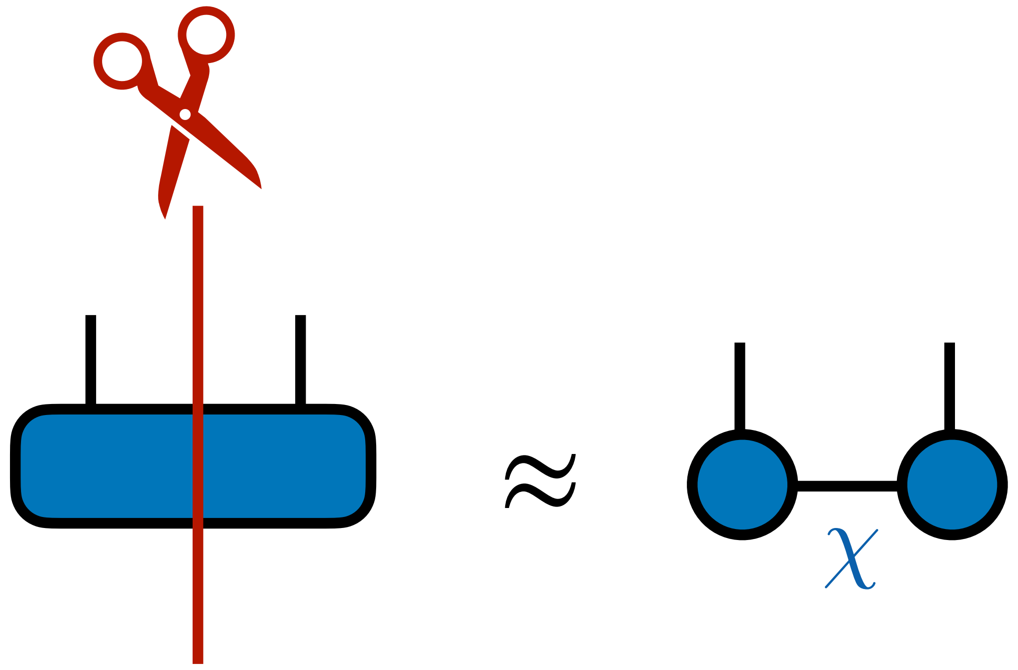
Low rank matrix



- Singular Value Decomposition (SVD) (or RRQR, RRLU …)

$$A = UDV \qquad D = \begin{pmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & \dots & 0 & \lambda_n \end{pmatrix}$$

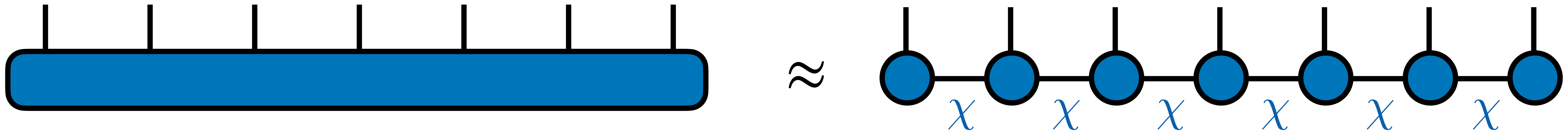
- Precision ϵ: keep χ largest singular values λ_i
- $\chi = \epsilon$-rank.



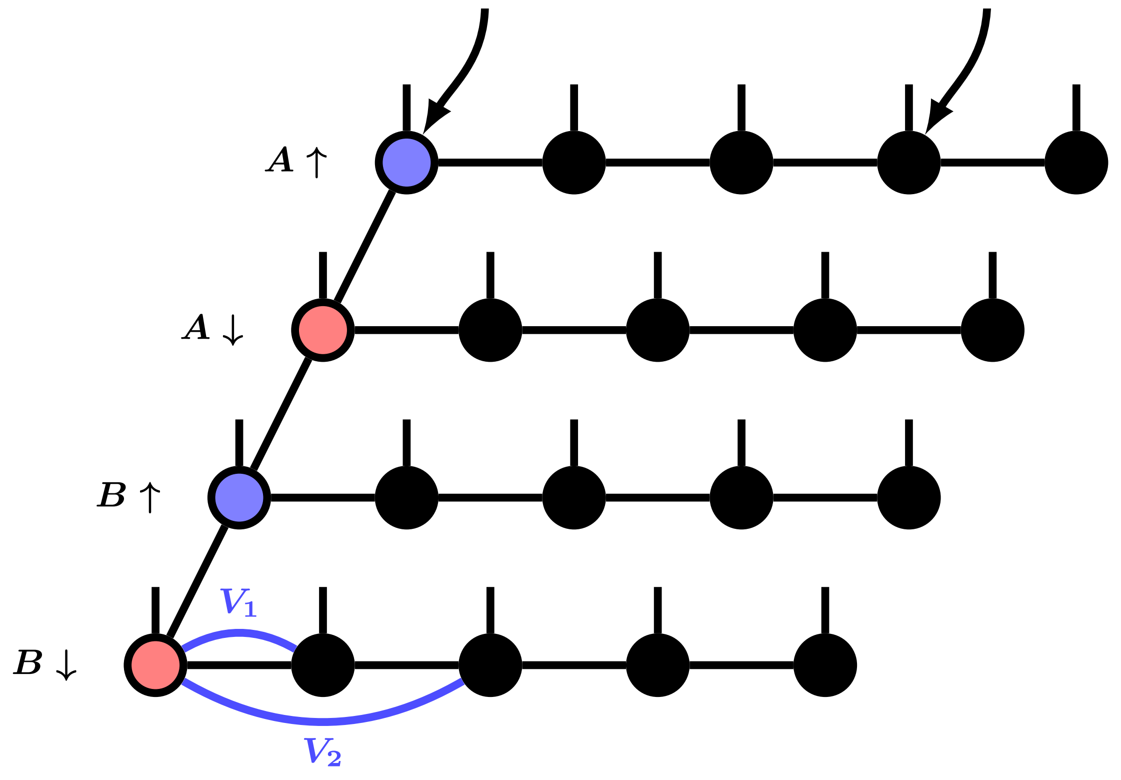
Low rank: save memory and computing time

Low rank tensors

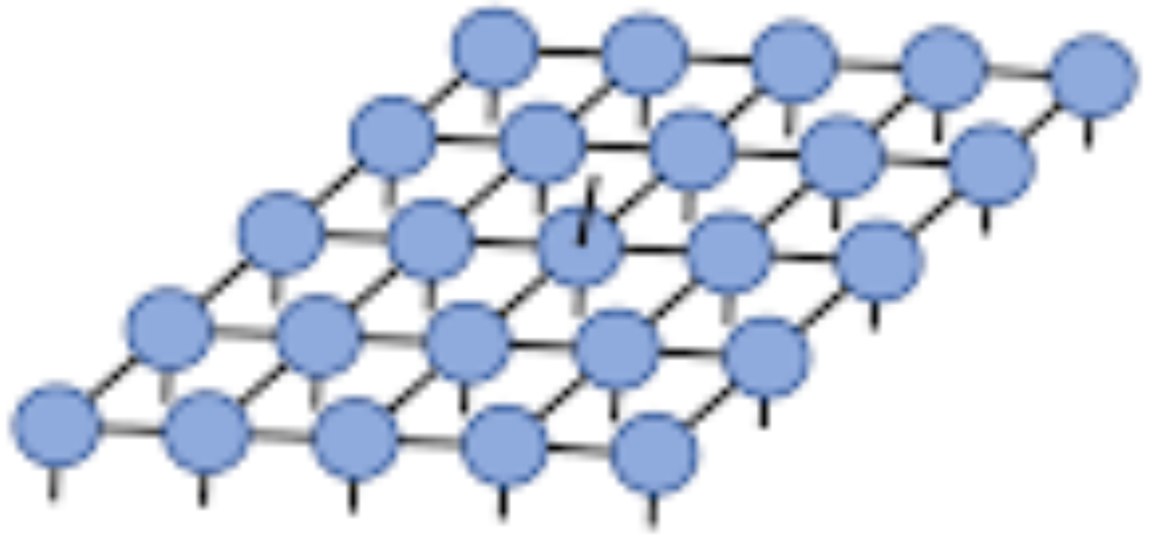
- Matrix product states (MPS) = Tensor Trains.



- Tree form



- 2D. PEPS, MERA, etc…

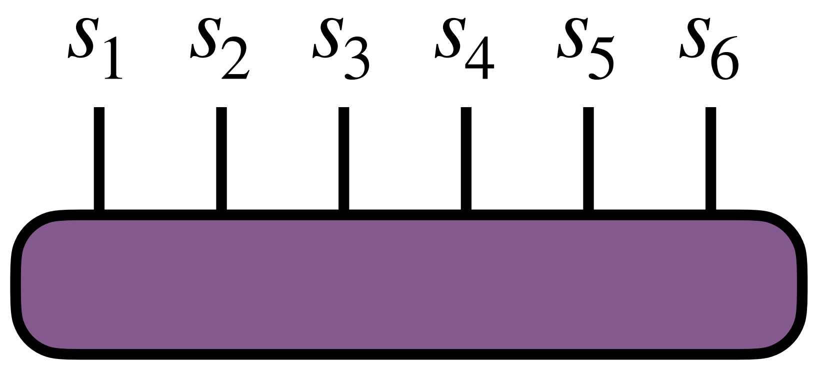


N-body wavefunctions

- Amplitudes are a tensor.

$$|\Psi\rangle = \sum_{s_1 s_2 s_3 \cdots s_n} \Psi(s_1, s_2, s_3, \cdots, s_n)\, |s_1 s_2 s_3 \cdots s_n\rangle$$

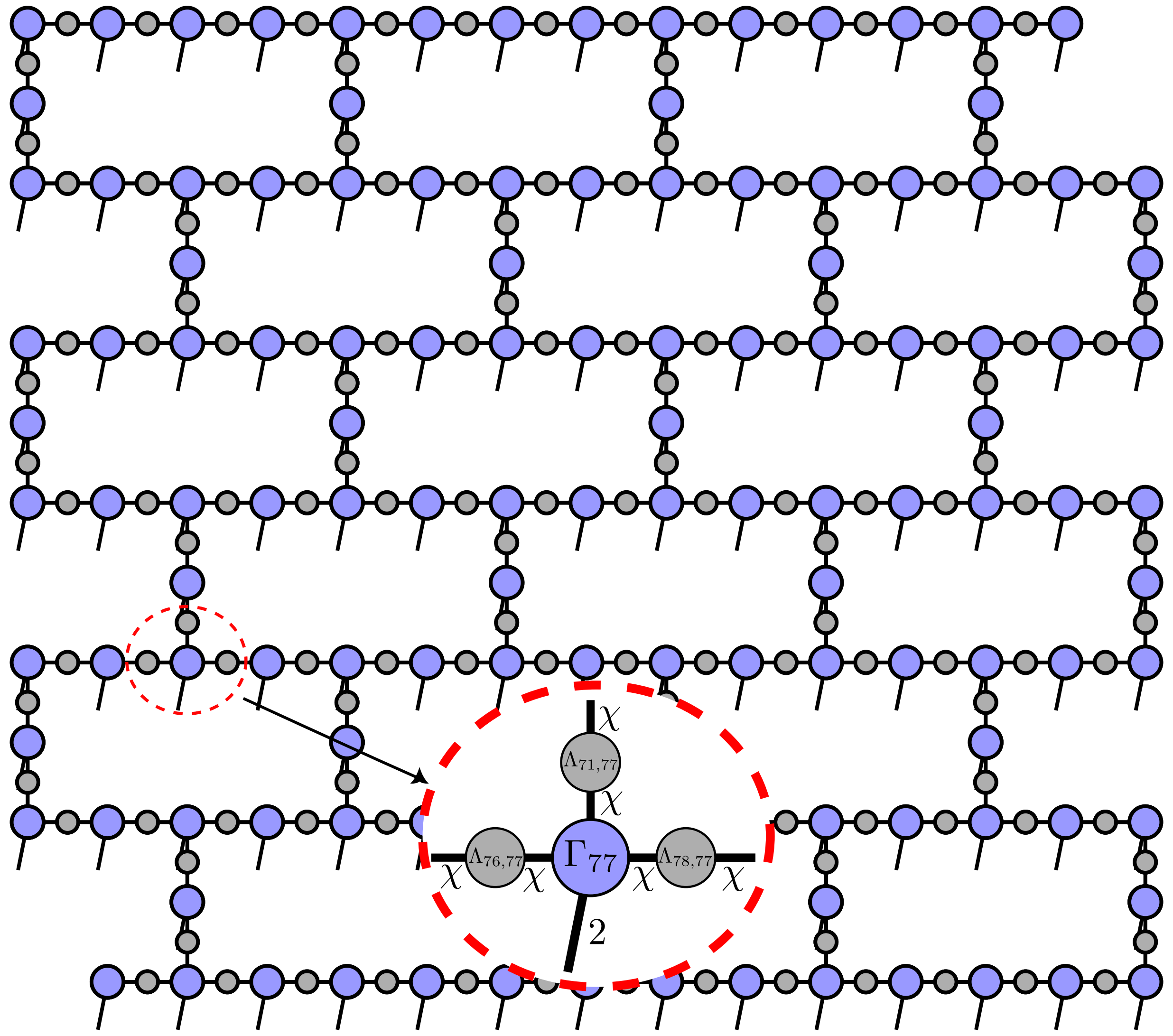
$$\Psi(s_1, s_2, s_3, s_4, s_5, s_6) =$$

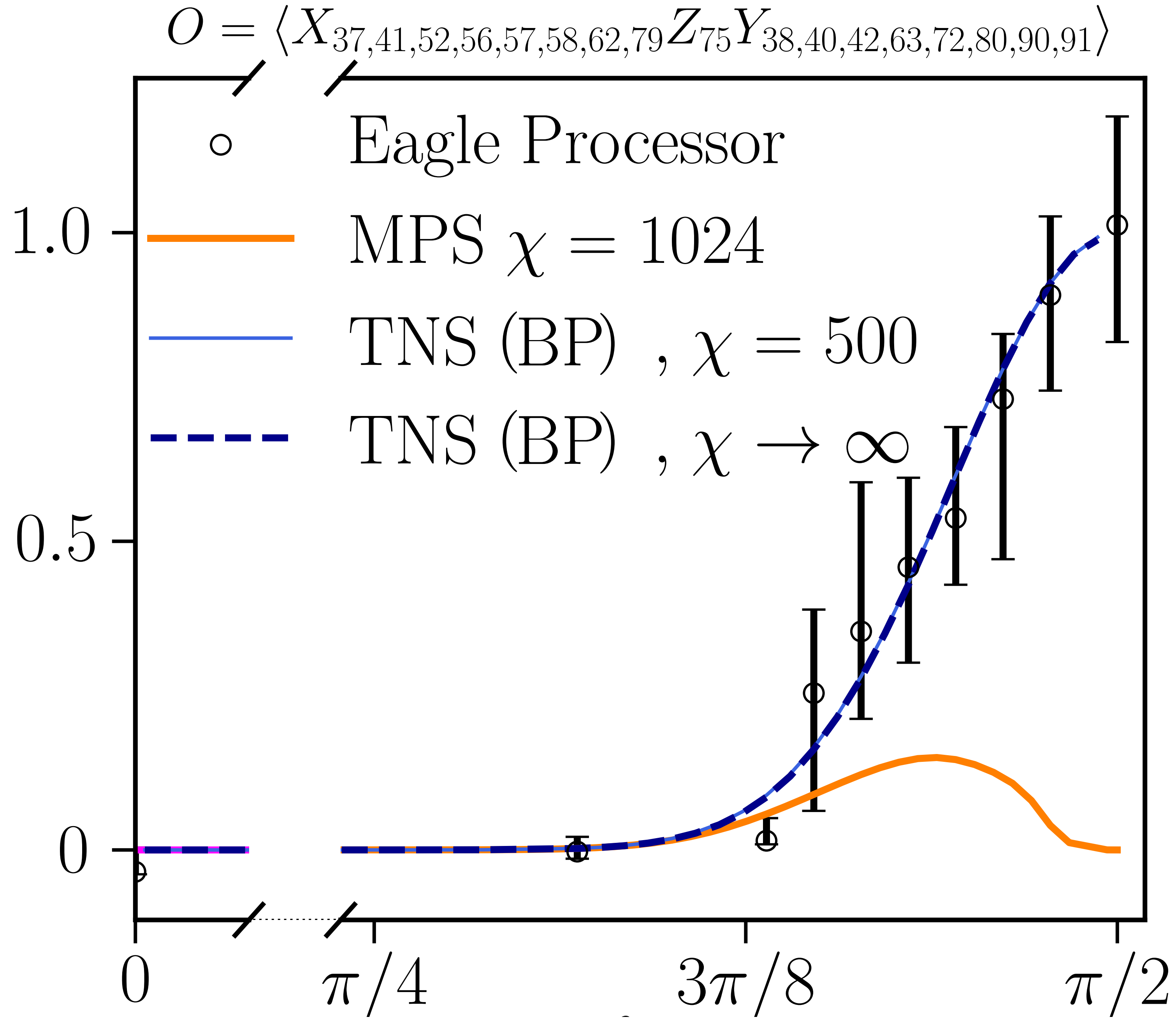


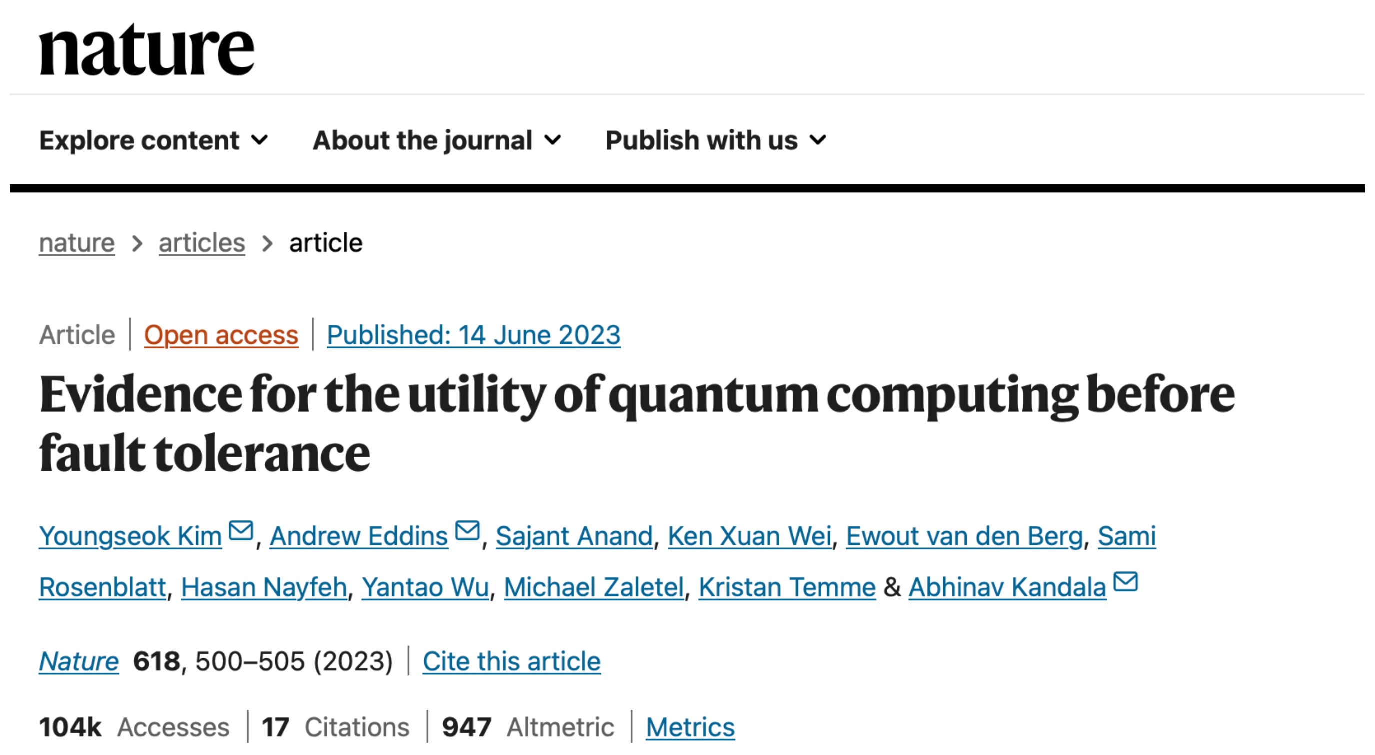
- Variational Ansatz for ground state Ψ_{GS} in term of a low rank tensor network.
- Controlled by quantum entanglement.
- Excellent for 1d systems. Harder for 2d systems (PEPS, MERA).

Simulating NISQ quantum computers

- Efficient tensor network simulation of IBM's Eagle kicked Ising experiment.
- No "quantum supremacy"







nature

Explore content ⌄ About the journal ⌄ Publish with us ⌄

nature > articles > article

Article | Open access | Published: 14 June 2023

Evidence for the utility of quantum computing before fault tolerance

Youngseok Kim, Andrew Eddins, Sajant Anand, Ken Xuan Wei, Ewout van den Berg, Sami Rosenblatt, Hasan Nayfeh, Yantao Wu, Michael Zaletel, Kristan Temme & Abhinav Kandala

Nature **618**, 500–505 (2023) | Cite this article

104k Accesses | **17** Citations | **947** Altmetric | Metrics

Joey Tindall

Matt Fishman

Dries Sels

Miles Stoudenmire

Tindall, Fishman, Stoudenmire, Sels arxiv:2306.14887
Tindall, Fishman, arxiv:2306.17837

Tensor Networks
for high dimensional integration

Large dimension integrals

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

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

- Curse of dimensionality : a priori $O(d^n)$.
- An ubiquitous problem e.g.
  - Partition functions.
  - Diagrammatics (real time, imaginary time).

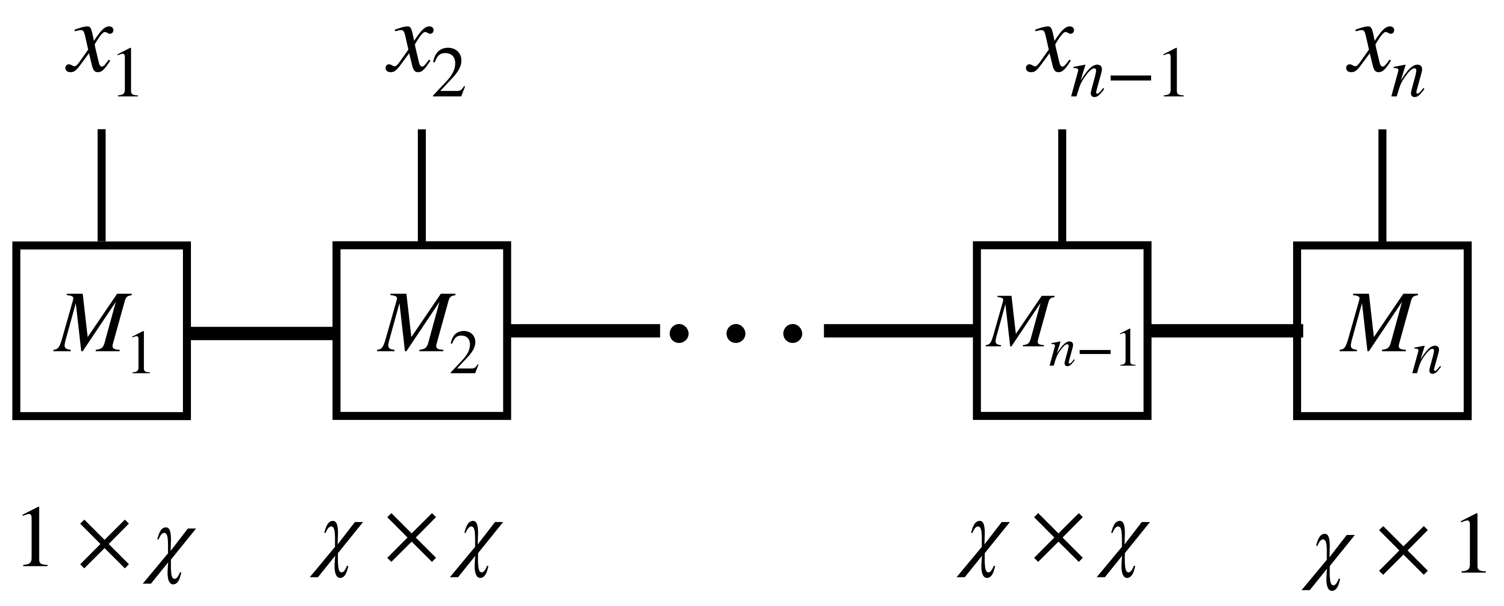
Compress to integrate

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) …

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

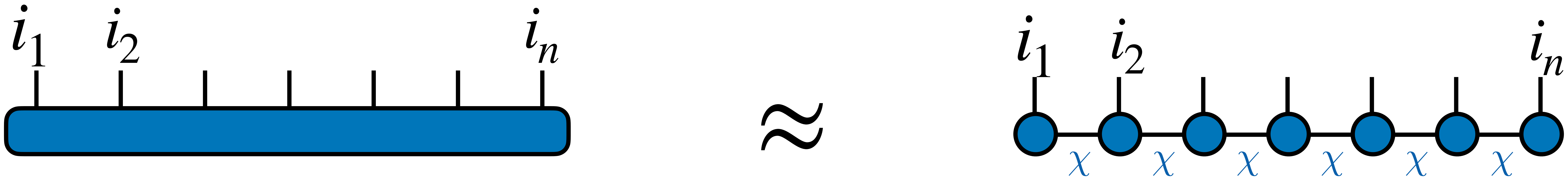


- with an error ε decreasing quickly with the rank χ (*ε-factorizable*) …
- then integration is reduced to 1d integrals. Almost separated variables.

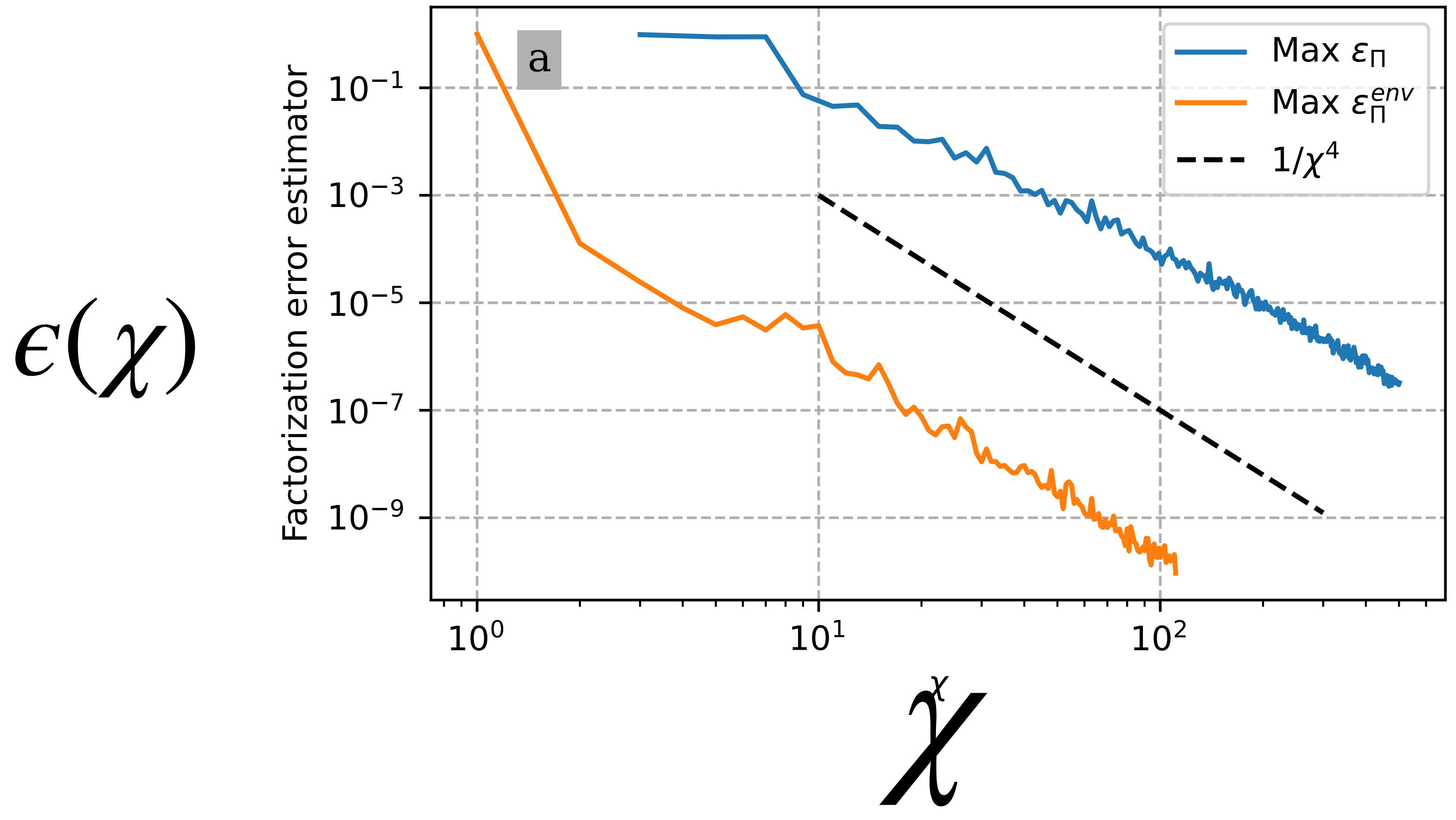
$$\int dx_1 \ldots dx_n \; f(x_1, \ldots, x_n) \approx \left(\int dx_1 M_1(x_1) \right) \ldots \left(\int dx_n M_n(x_n) \right)$$

Tensor Cross Interpolation (TCI) algorithm

*I. **Oseledets and E. Tyrtyshnikov**, Linear Algebra and its Applications 432, 70 (2010).*
***S. Dolgov and D. Savostyanov**, Computer Physics Communications 246, 106869 (2020)*



- Builds MPS approximation for $T_{i_1,i_2,\ldots,i_n}$, with $i_k \in \{1,\ldots,d\}$
- Evaluating T on only $N \sim nd\chi^2 \ll d^n$ points.
- Error estimator $\epsilon(\chi)$, decreasing with rank/bond dimension χ
- Rank Revealing algorithm



A concrete example

Perturbative series

Phys Rev X 12, 041018 (2022)

Collaborators : Ph. Dumitrescu, Y. Nuñez-Fernandez, X. Waintal, J. Kaye

Perturbative series

- In equilibrium ("Diagrammatic Quantum Monte Carlo")

From Prokofiev, Svistunov 98,
Many works in equilibrium
e.g. Hubbard model, pseudogap:
Simkovic et al. arXiv:2209.09237

- Here, real time, out of equilibrium (Schwinger-Keldysh).

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

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

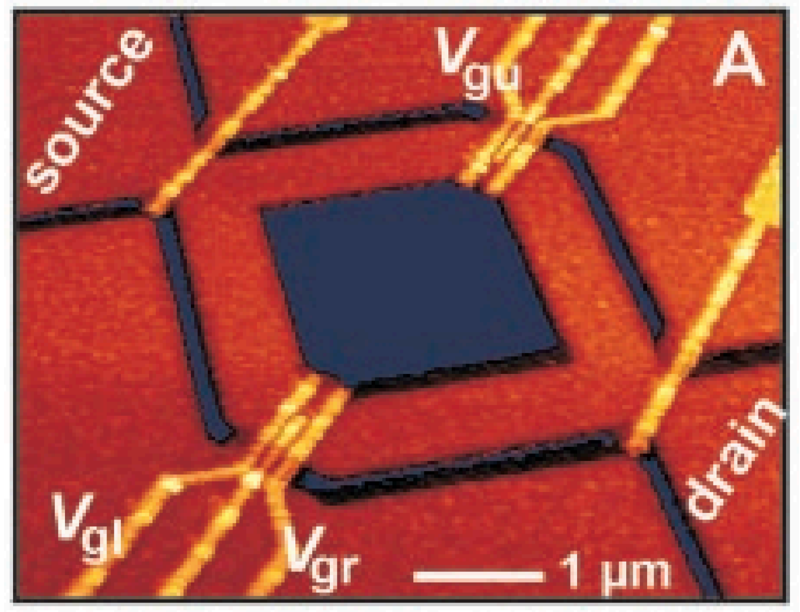
Time

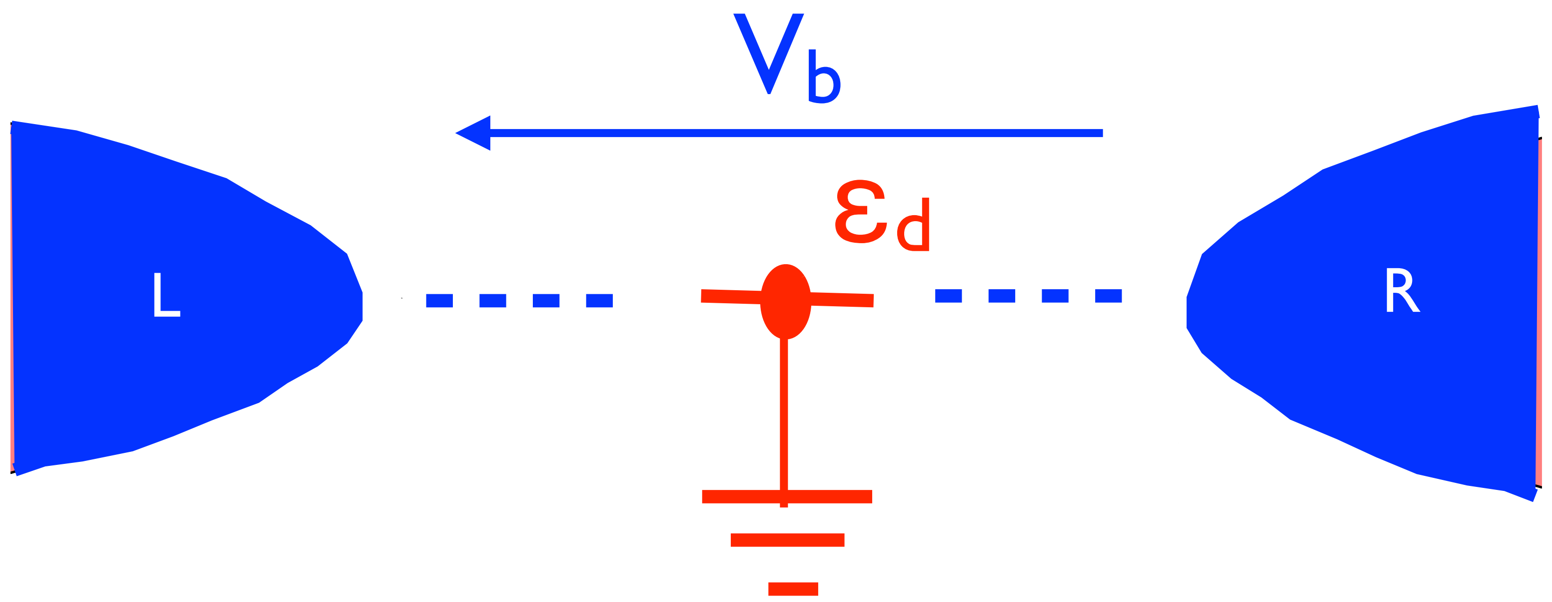
Interaction

- Even in strong coupling regime (e.g. Kondo effect, pseudo gap in Hubbard model)
- Beyond the finite radius of convergence of the series, using resummation techniques.

A concrete case: quantum dot

- Anderson model, 2 leads (L, R).





Bath *Dot* *Hybridization*

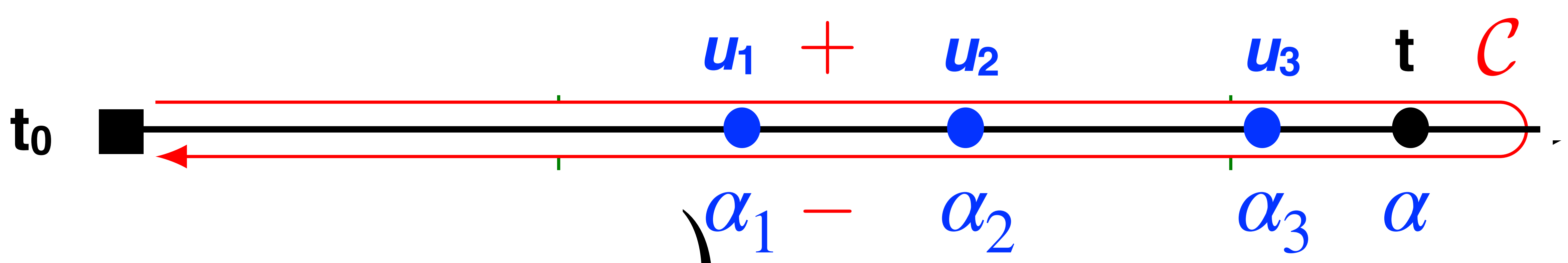
$$H = \sum_{\substack{k\sigma \\ \alpha=L,R}} \varepsilon_{k\alpha} c^\dagger_{k\sigma\alpha} c_{k\sigma\alpha} + \sum_{\sigma} \varepsilon_d d^\dagger_\sigma d_\sigma + U n_{d\uparrow} n_{d\downarrow} + \sum_{\substack{k\sigma \\ \alpha=L,R}} g_{k\sigma\alpha} (c^\dagger_{k\sigma\alpha} d_\sigma + h.c.)$$

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

- Schwinger-Keldysh

Switch on interaction

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



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

Monte Carlo
or Tensor network …

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

- q_n costs $O(2^n)$ to evaluate. We compute up to 30 orders.

q_n is ε-factorizable !

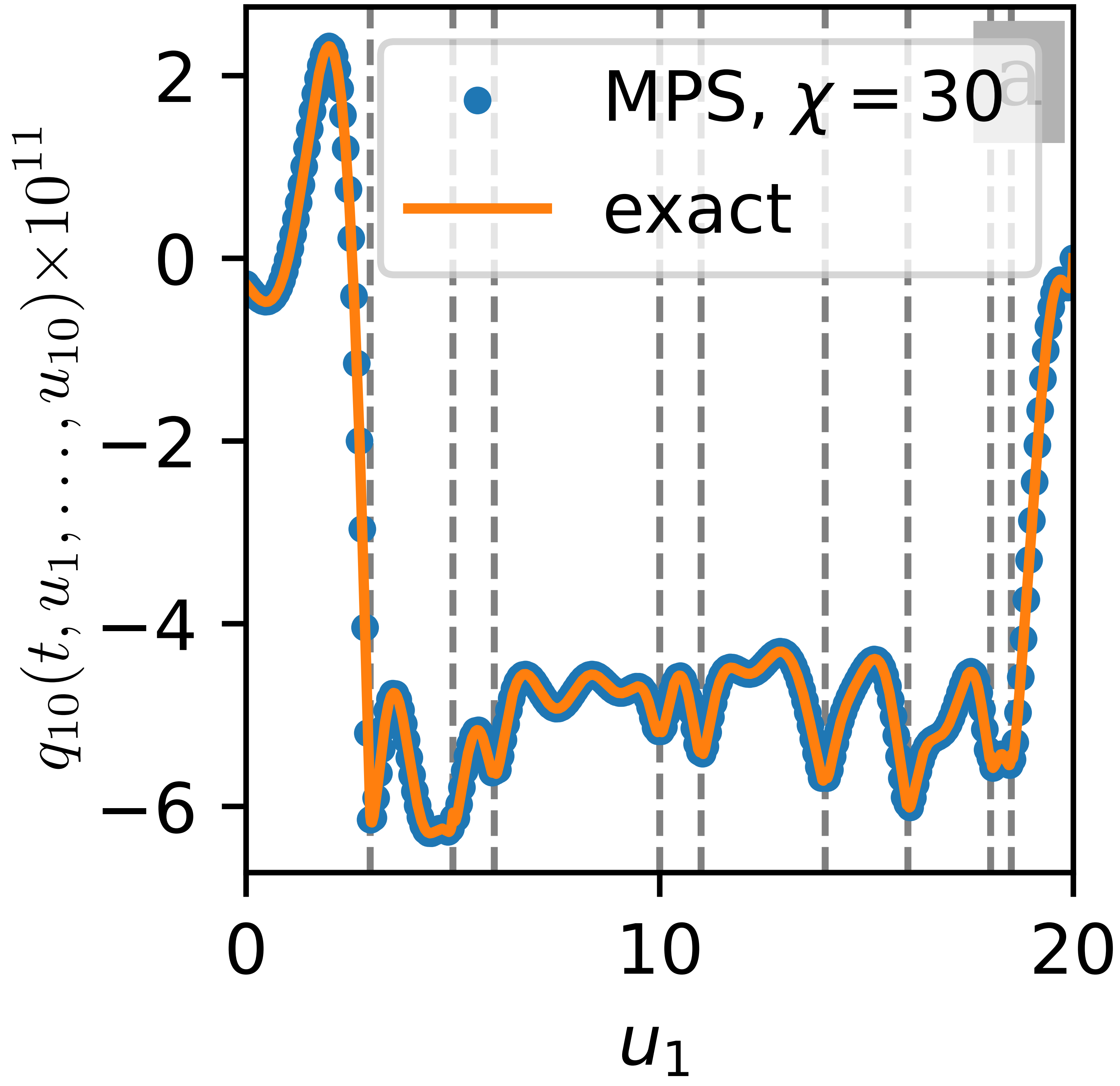
- In the time differences v_i. (with time-ordered u_i)

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

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

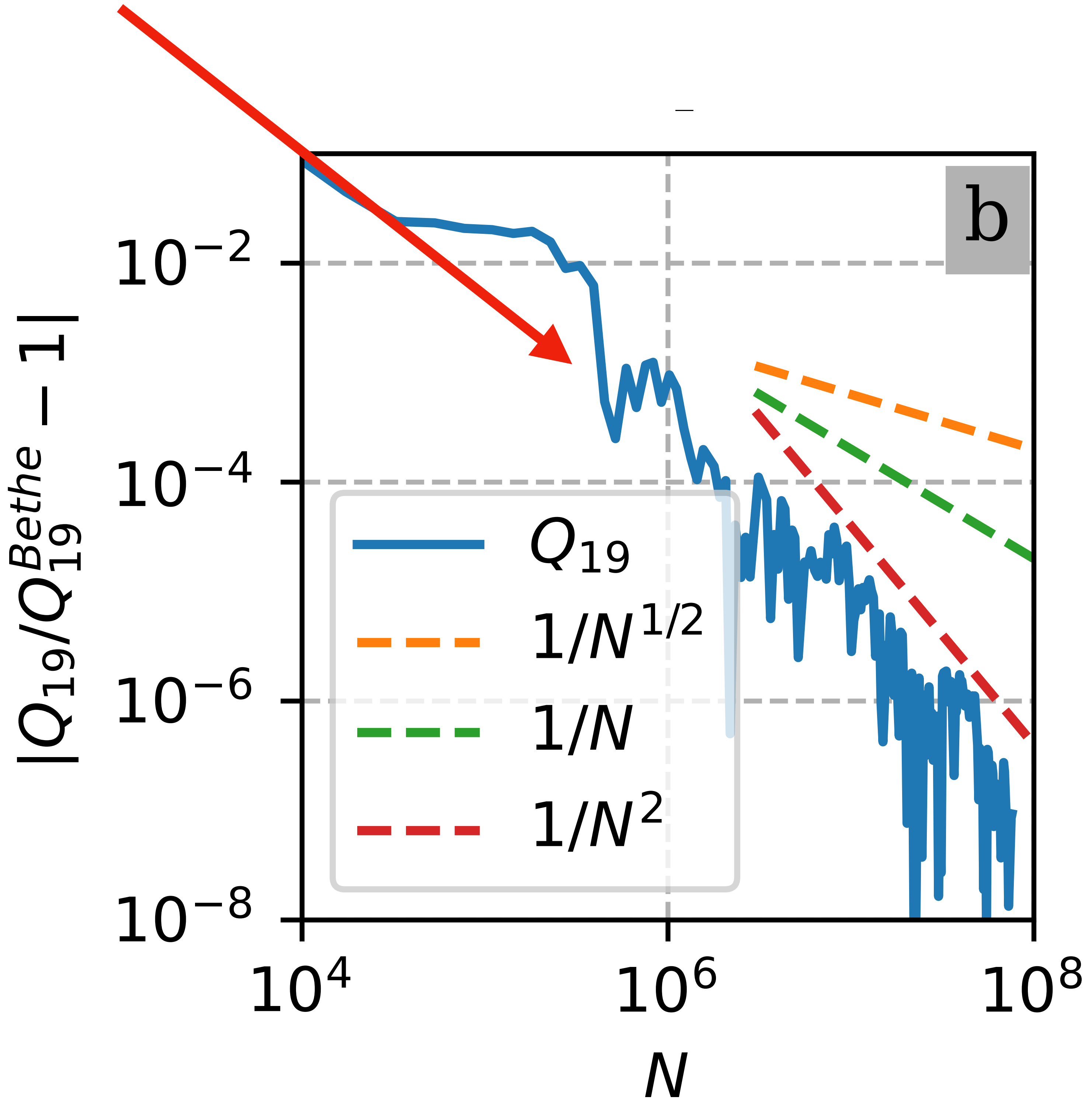
- Decompose q_n with TCI and integrate

Charge of the dot,
q_{10} vs its MPS interpolation

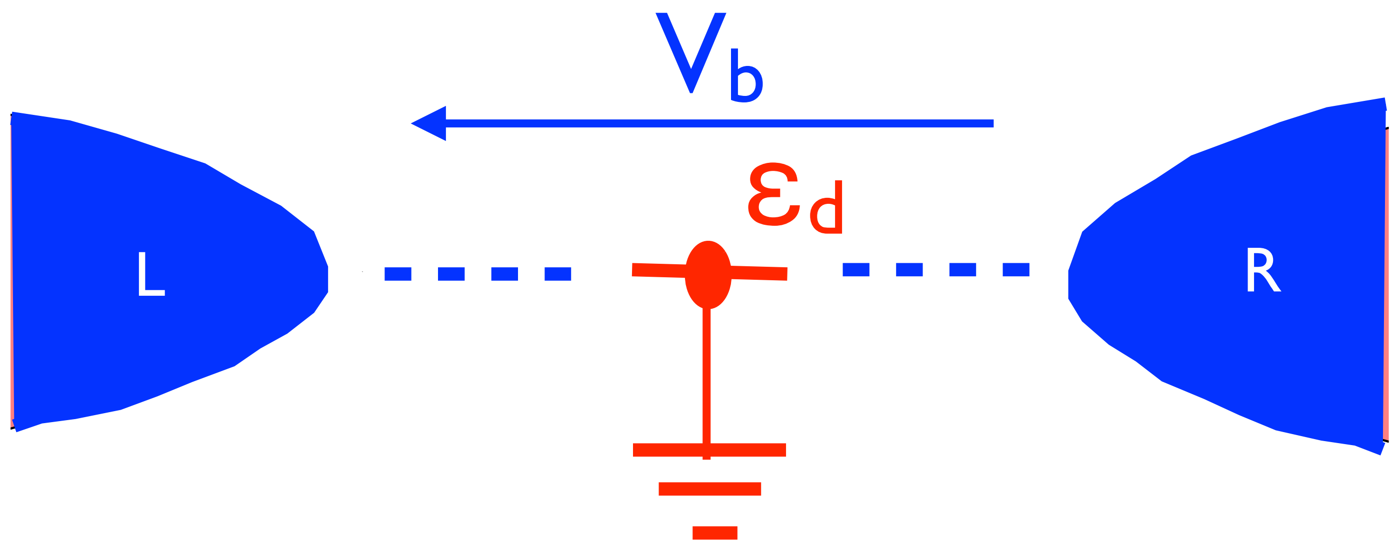


Benchmark

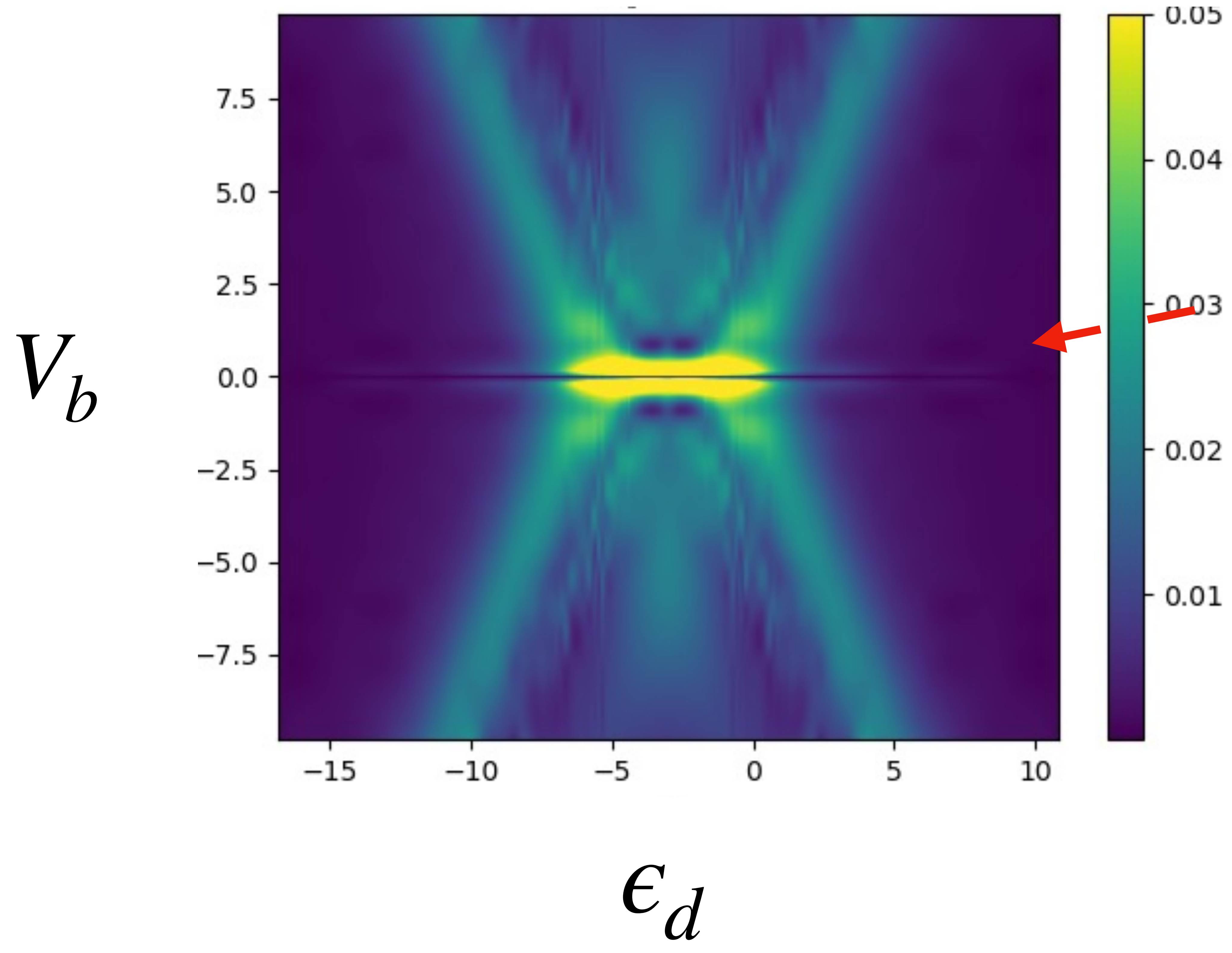
- High precision (9 digits) benchmark vs integrable case (equilibrium, flat bath).
- Number of evaluations of q_n : $N \sim \chi^2$
- χ does not grow with n
- Convergence rate : error $\sim 1/N^2$

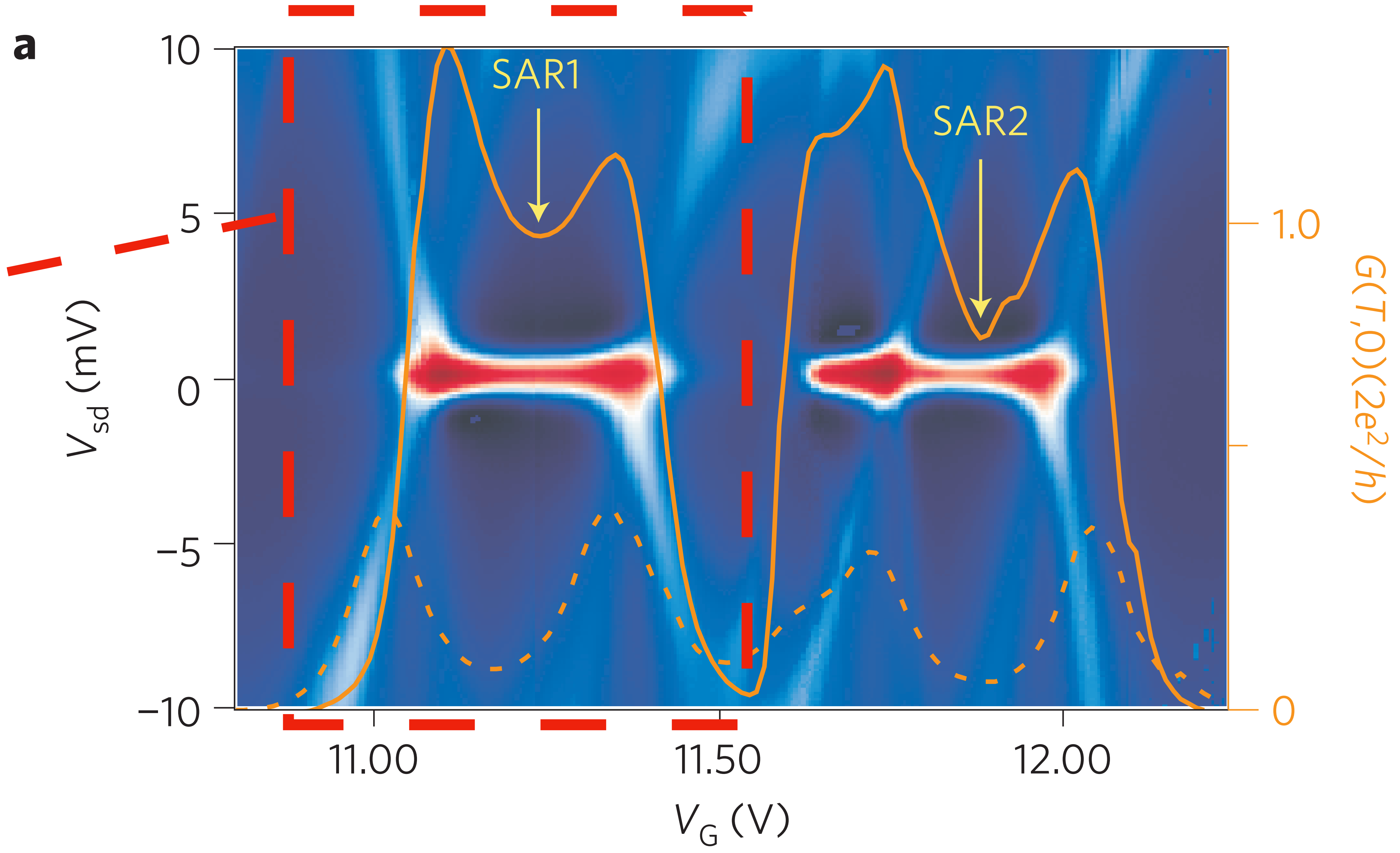


Differential conductance



$$G \equiv \frac{\partial I}{\partial V_b} \qquad U = 6$$





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

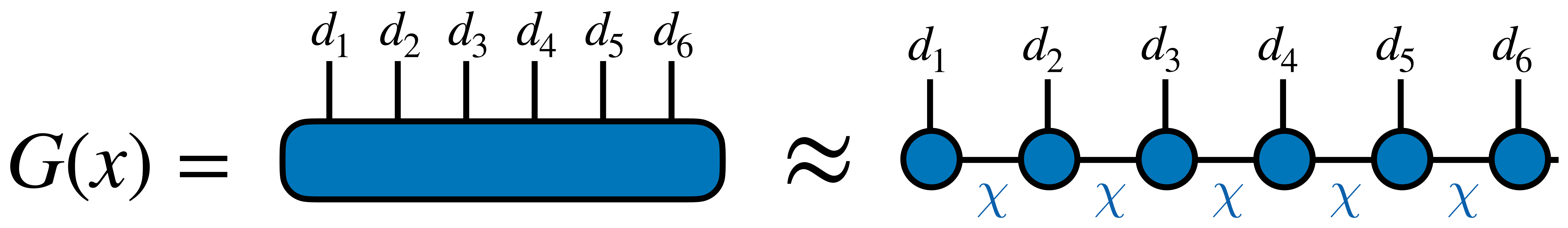
Computation

What about one (or few) variables functions ?

Quantics tensor trains (QTT)

- Function of **one** continuous variable x as a tensor

$$0 \leq x < 1 \qquad\qquad x = 0.d_1 d_2 d_3 d_4 d_5 d_6$$

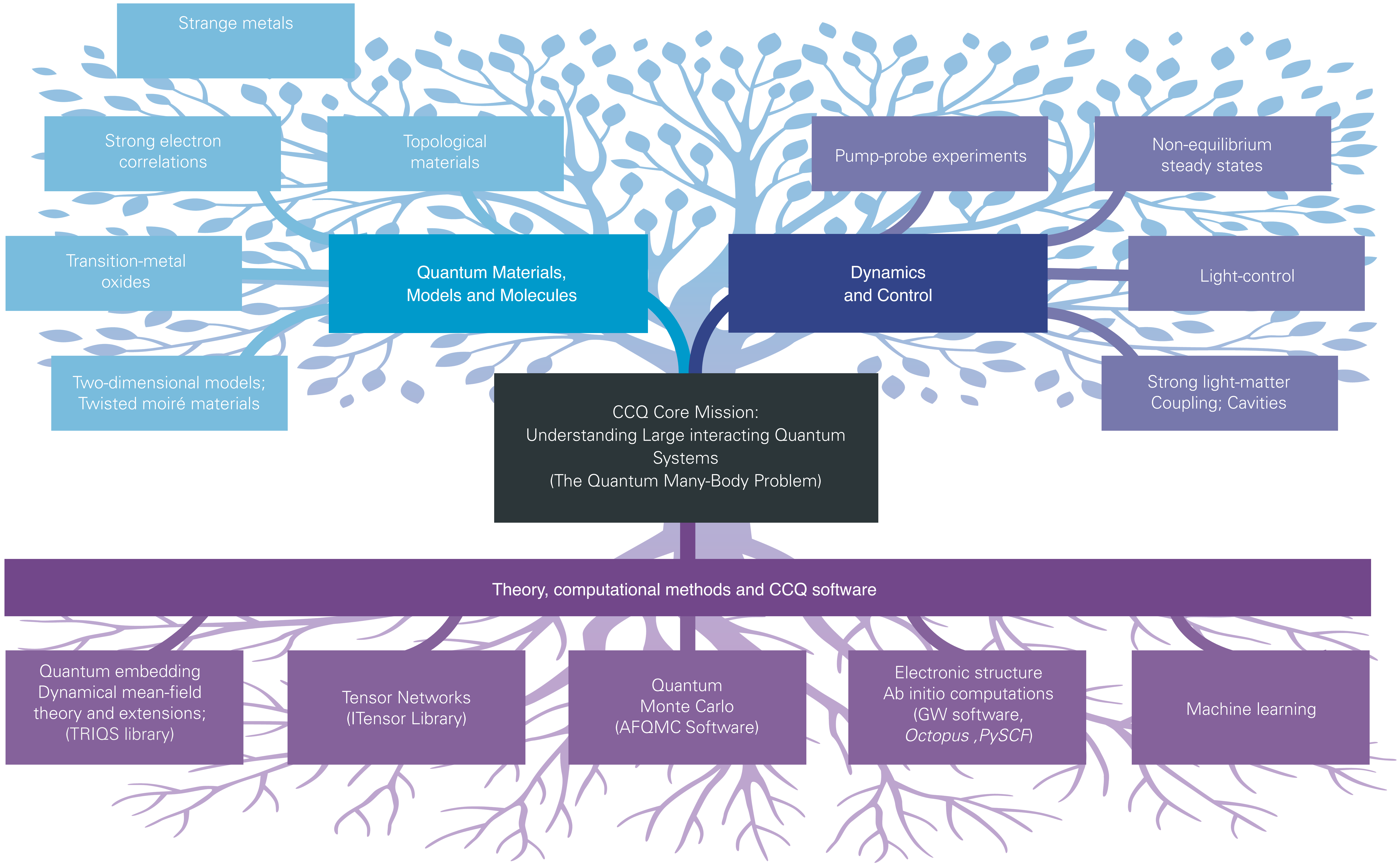


$$d_j = 0, 1, 2, \ldots, 9$$

- Many functions have low rank χ (e.g. e^x has rank 1).
- Manipulate G in this representation, similar to orthogonal polynomials.
- Many potential applications e.g. PDE, turbulence, …

(Usually use base 2 though, for example $1/3 \approx 0.01010101$)

The CCQ Research Ecosystem



Strange metals

Strong electron correlations

Topological materials

Transition-metal oxides

Two-dimensional models; Twisted moiré materials

Quantum Materials, Models and Molecules

Pump-probe experiments

Non-equilibrium steady states

Light-control

Strong light-matter Coupling; Cavities

Dynamics and Control

CCQ Core Mission:
Understanding Large interacting Quantum Systems
(The Quantum Many-Body Problem)

Theory, computational methods and CCQ software

Quantum embedding Dynamical mean-field theory and extensions; (TRIQS library)

Tensor Networks (ITensor Library)

Quantum Monte Carlo (AFQMC Software)

Electronic structure Ab initio computations (GW software, *Octopus* ,*PySCF*)

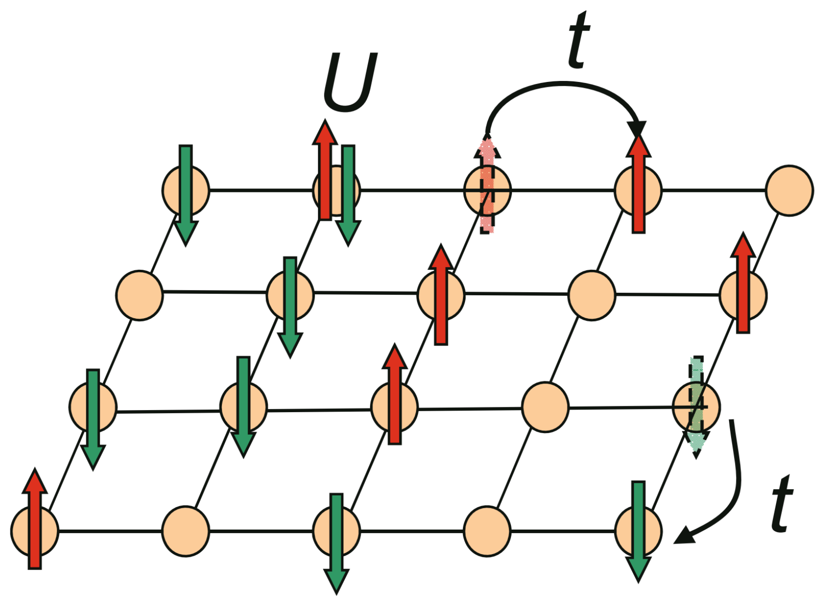
Machine learning

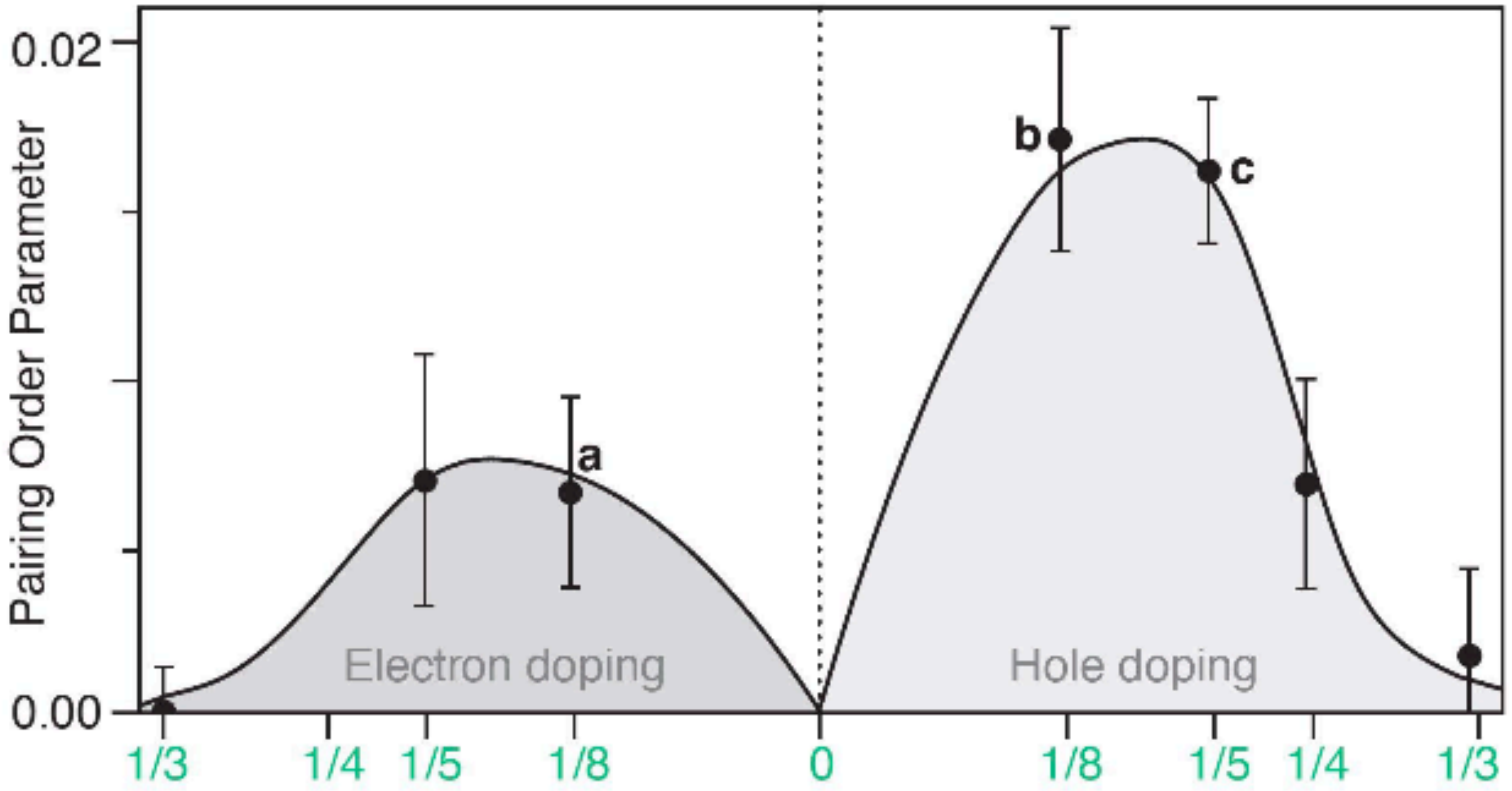
Auxiliary field QMC

Hubbard model has high-Tc d-SC superconductivity

- With second neighbor hopping
- AFQMC & DMRG

Shiwei Zhang (CCQ)





arXiv:2303.0837 March 15, 2023

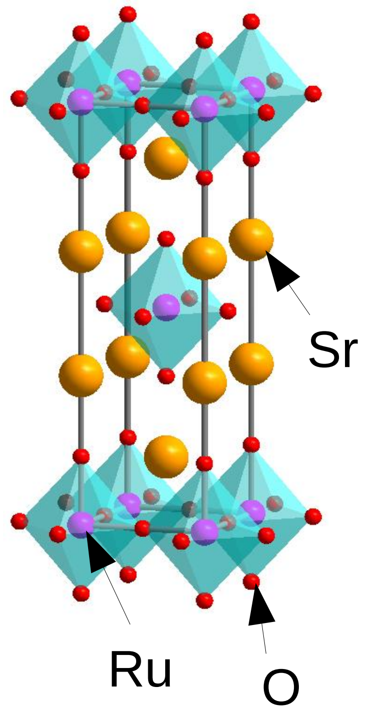
Coexistence of superconductivity with partially filled stripes in the Hubbard model

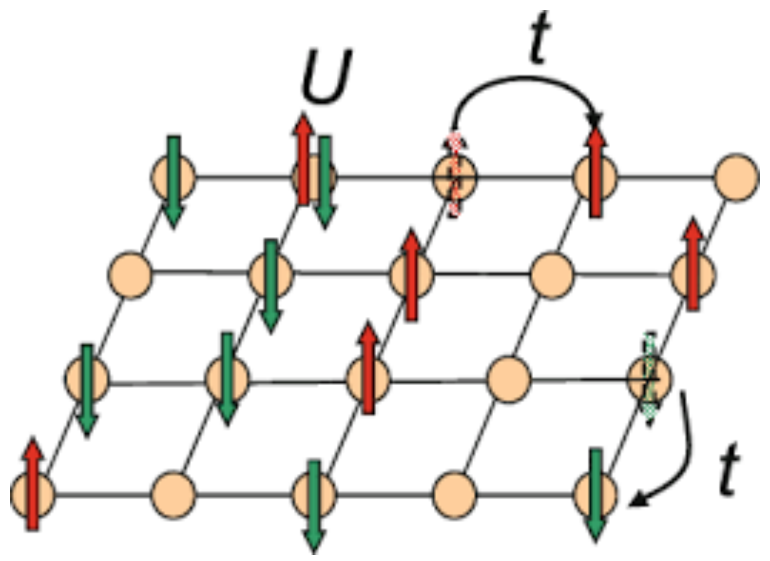
Hao Xu,[1,*] Chia-Min Chung,[2,3,4,*] Mingpu Qin,[5] Ulrich Schollwöck,[6,7] Steven R. White,[8] and Shiwei Zhang[9]

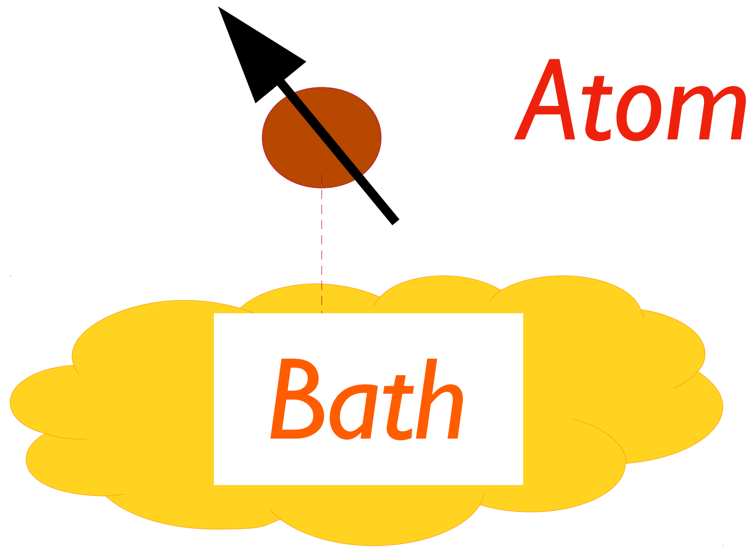
Quantum Embeddings

Quantum Embeddings

Dynamical Mean Field Theory (DMFT) and beyond,
A. Georges, G. Kotliar 92.



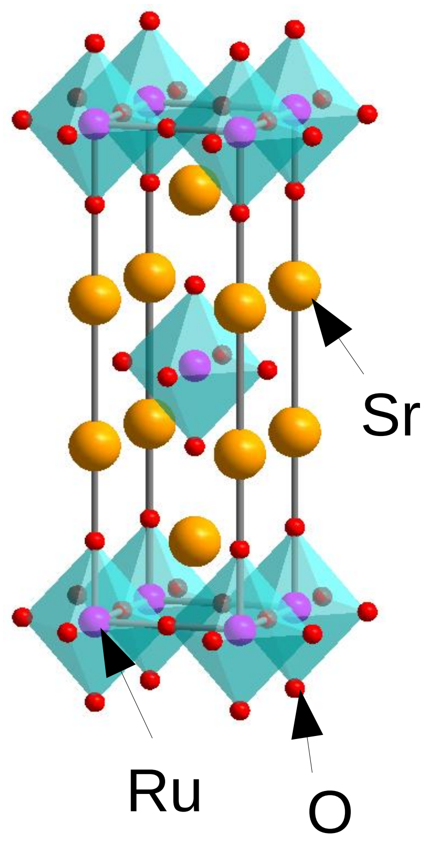




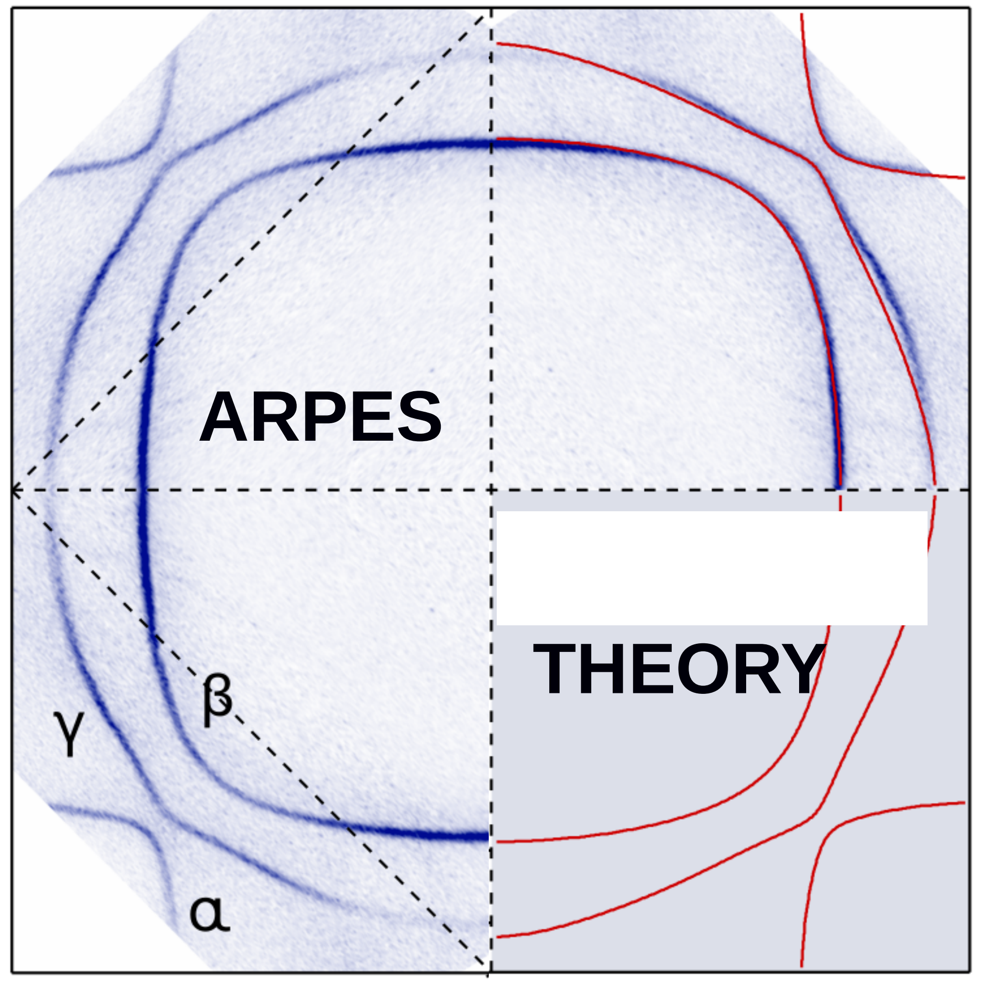
Auxiliary
"Quantum impurity" model

A few degrees of freedoms
(d/f-shell)
coupled to a non-interacting
self-consistently bath of fermions

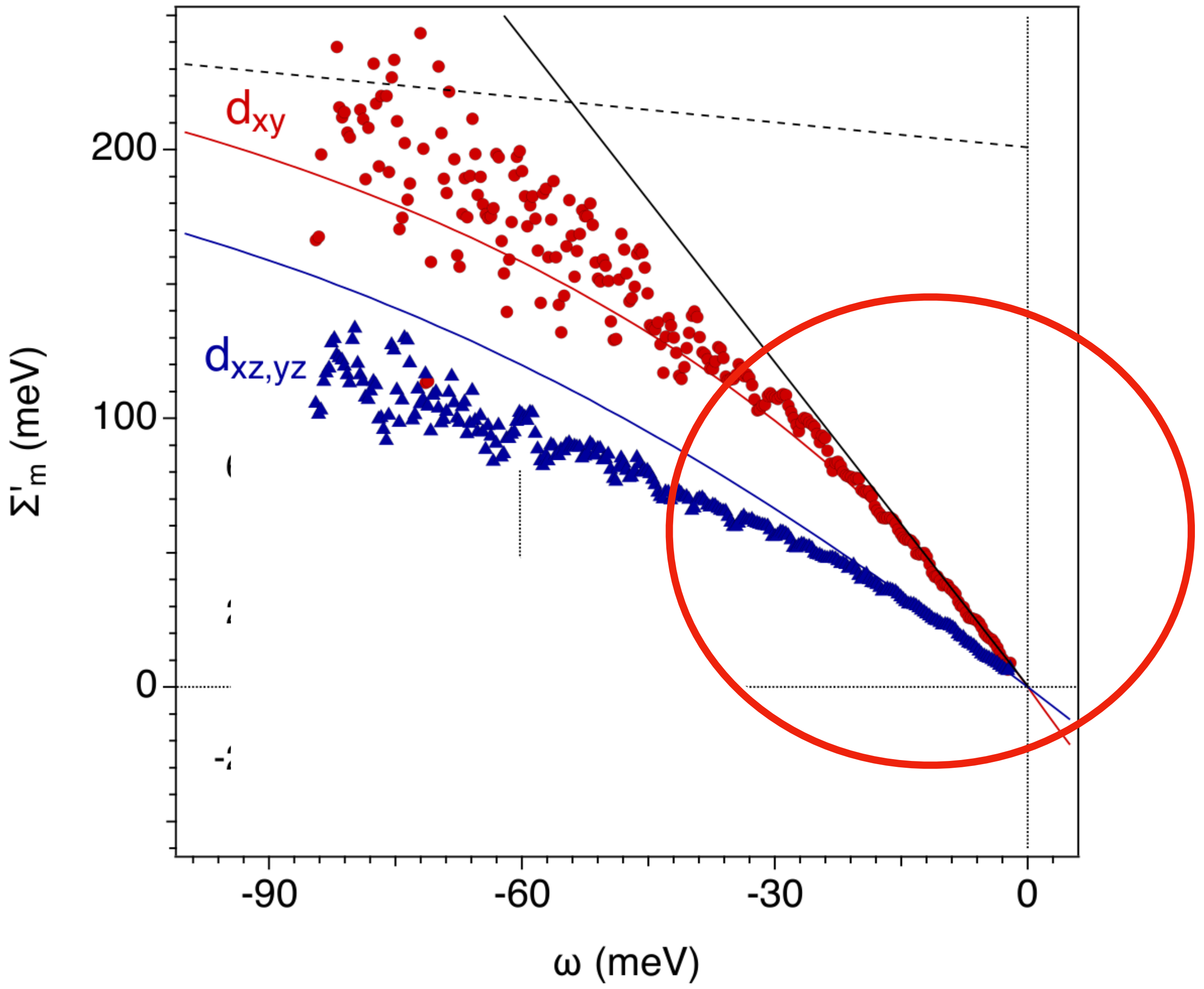
Sr_2RuO_4, a correlated Hund’s metal



- Normal phase. Great comparison with experiments.

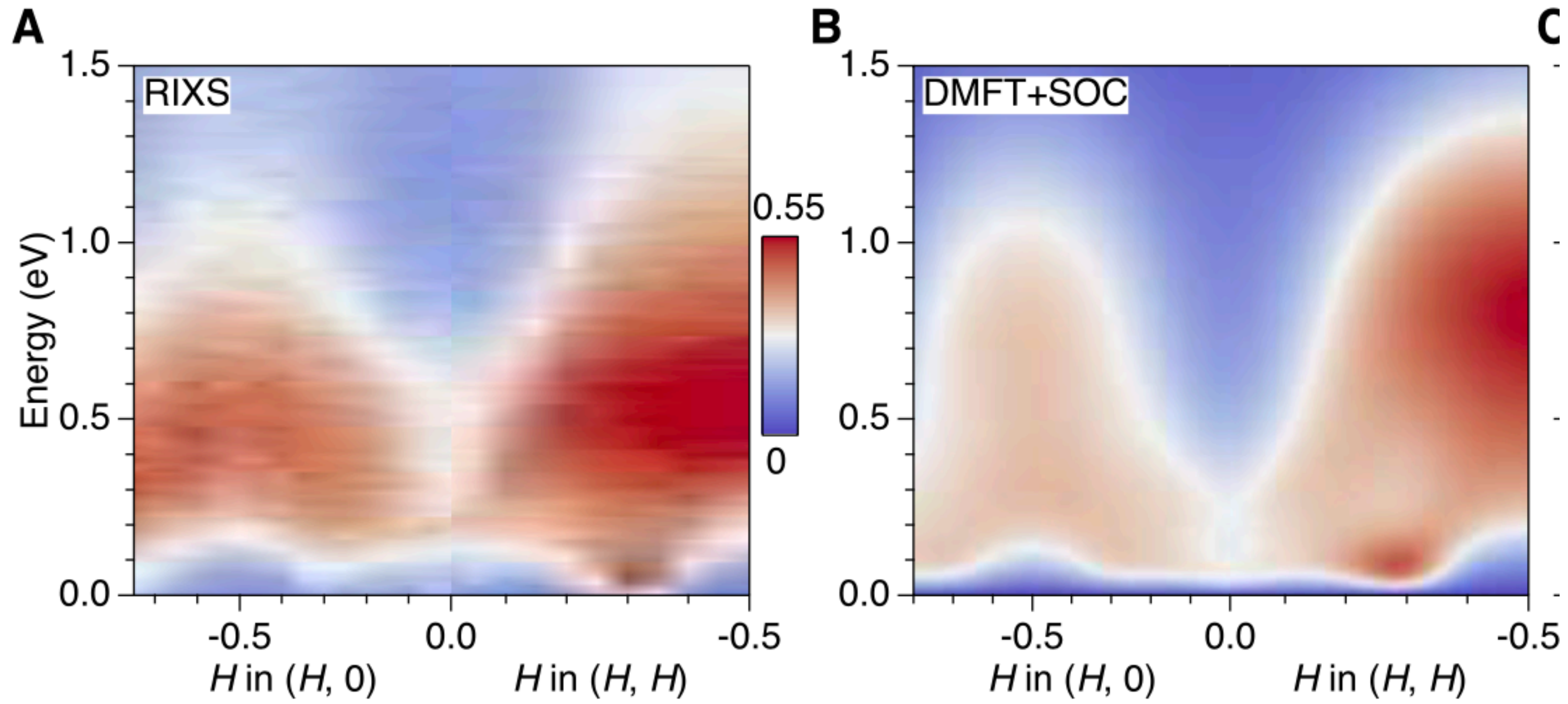


Fermi surface



Self-energy

A. Tamai, M. Zingl et al.
Phys. Rev. X 9, 021048 (2019)



Spin Dynamics (RIXS)

H. Suzuki et al.,
Nat. Commun. 14, 7042 (2023)

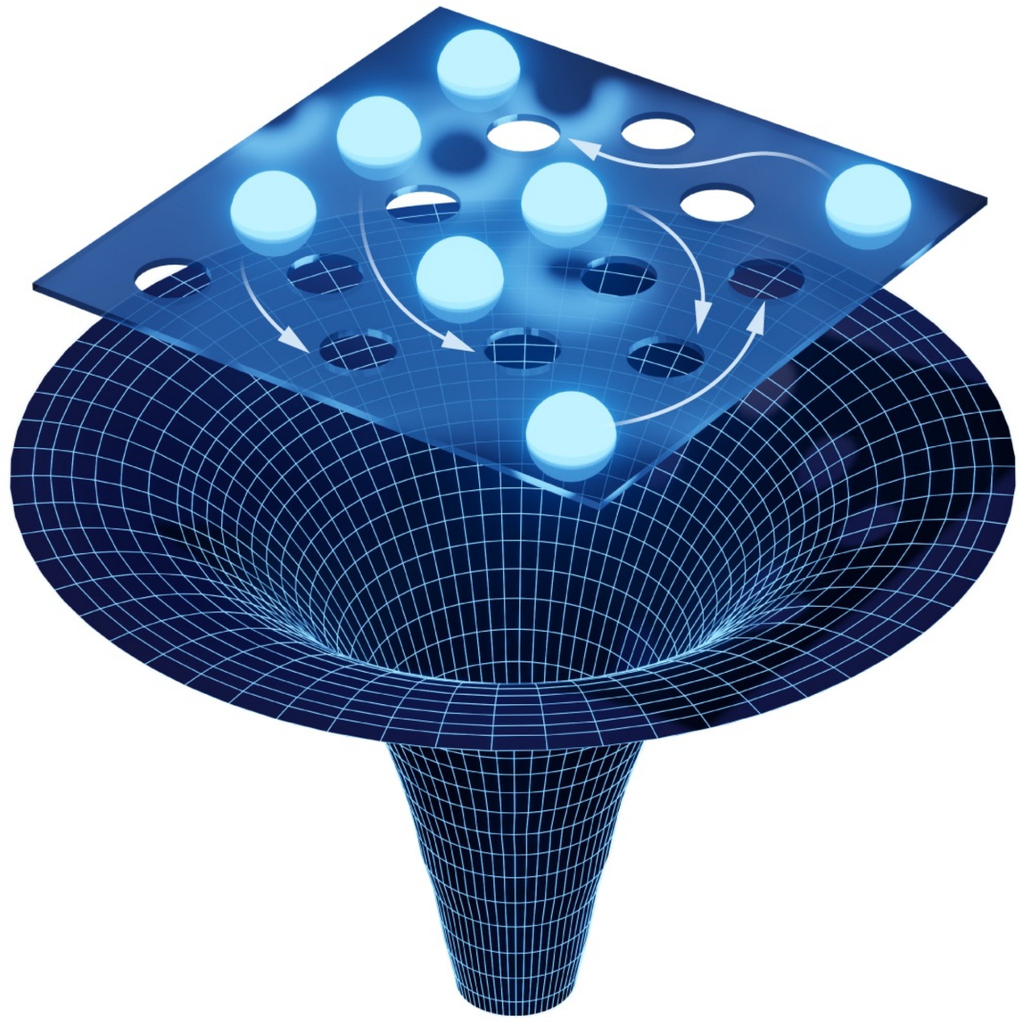
- Superconducting phase. Order ? Mechanism ?

Planckian metal

D. Chowdhury, A. Georges, O.P., S. Sachdev
Rev. Mod. Phys. 94, 035004 (2022)

- A class of non Fermi liquid metals.
  - No quasi-particles.
  - Relaxation time is minimal
  - T-linear resistivity down to T=0

$$\tau \sim \frac{\hbar}{k_B T}$$



- SYK (Sachdev-Ye-Kitaev) models
  - A family of non Fermi liquids without quasi-particles.
  - Holography. AdS-CFT correspondance.

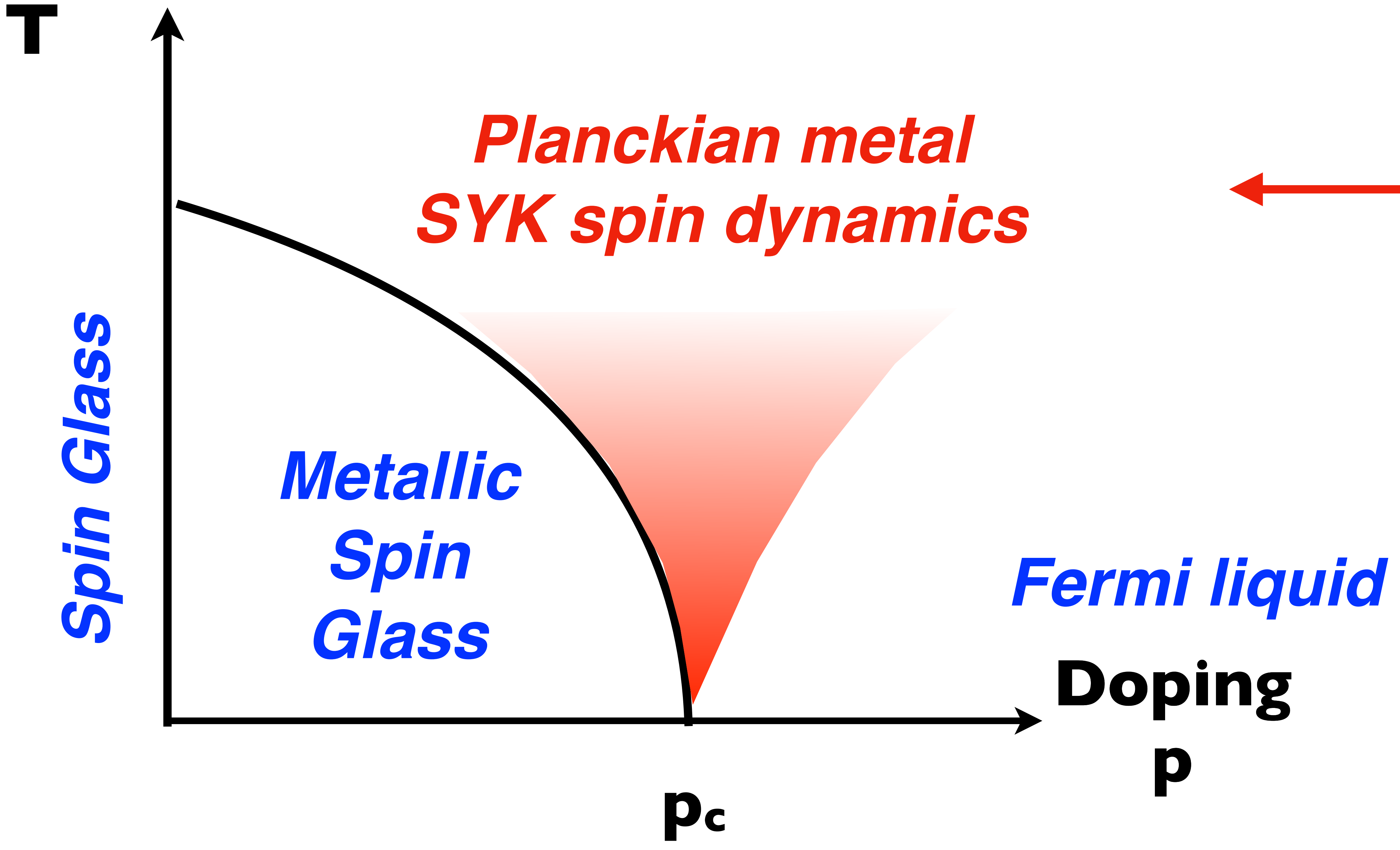
Doped quantum spin glass

Ph. Dumitrescu, N. Wentzell, A. Georges, OP Phys. Rev. B 2022

- SU(2) disordered Heisenberg model + holes

$$H = -\sum_{ij,\sigma}(t_{ij} + \mu\delta_{ij})c^{\dagger}_{i\sigma}c_{j\sigma} + \sum_{i<j} J_{ij}\boldsymbol{S}_i \cdot \boldsymbol{S}_j + U\sum_i n_{i\uparrow}n_{i\downarrow},$$

Philipp Dumitrescu (CCQ)



- Slow spin dynamics.
- Linear resistivity at the quantum critical point

$$\rho \sim T$$

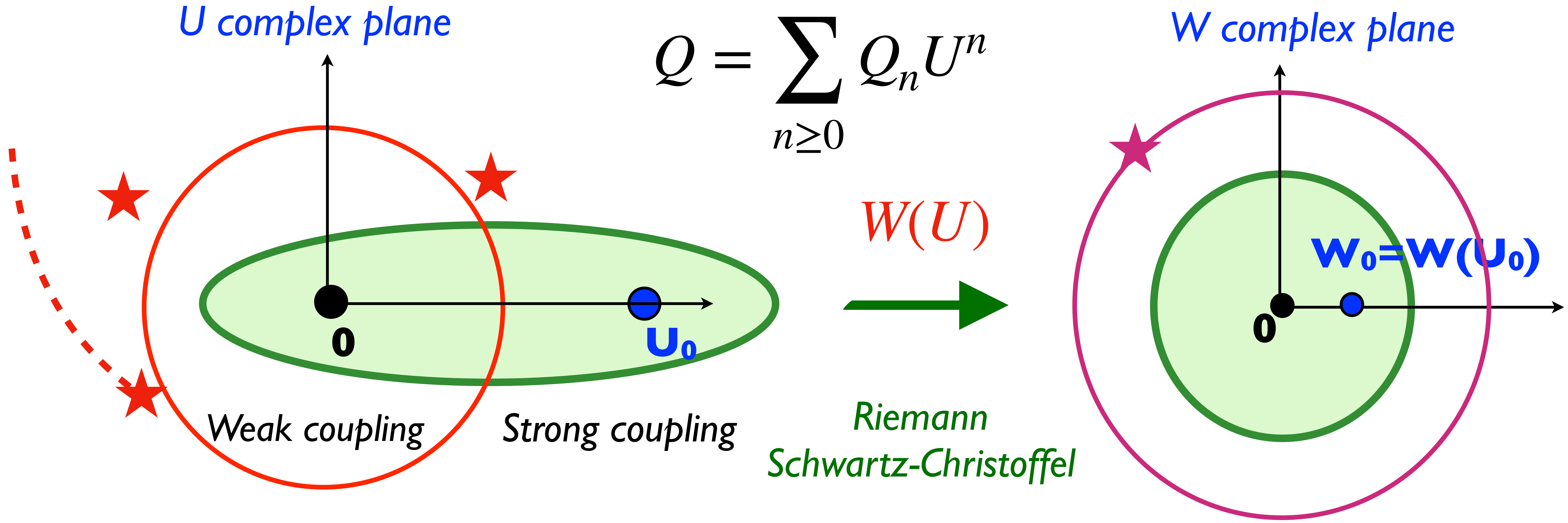
- Transport time close to the Planckian limit

$$\frac{1}{\tau_{\mathrm{tr}}} \simeq c\frac{k_B T}{\hbar}$$

Thank you for your attention!

Conformal change of variables

Profumo et al. PRB 91, 245154 (2015)
Bertrand et al. Phys. Rev. X 9, 041008 (2019)



$$Q = \sum_{n\geq 0} Q_n U^n$$

A finite radius of convergence !
Singularities poles, branch cuts

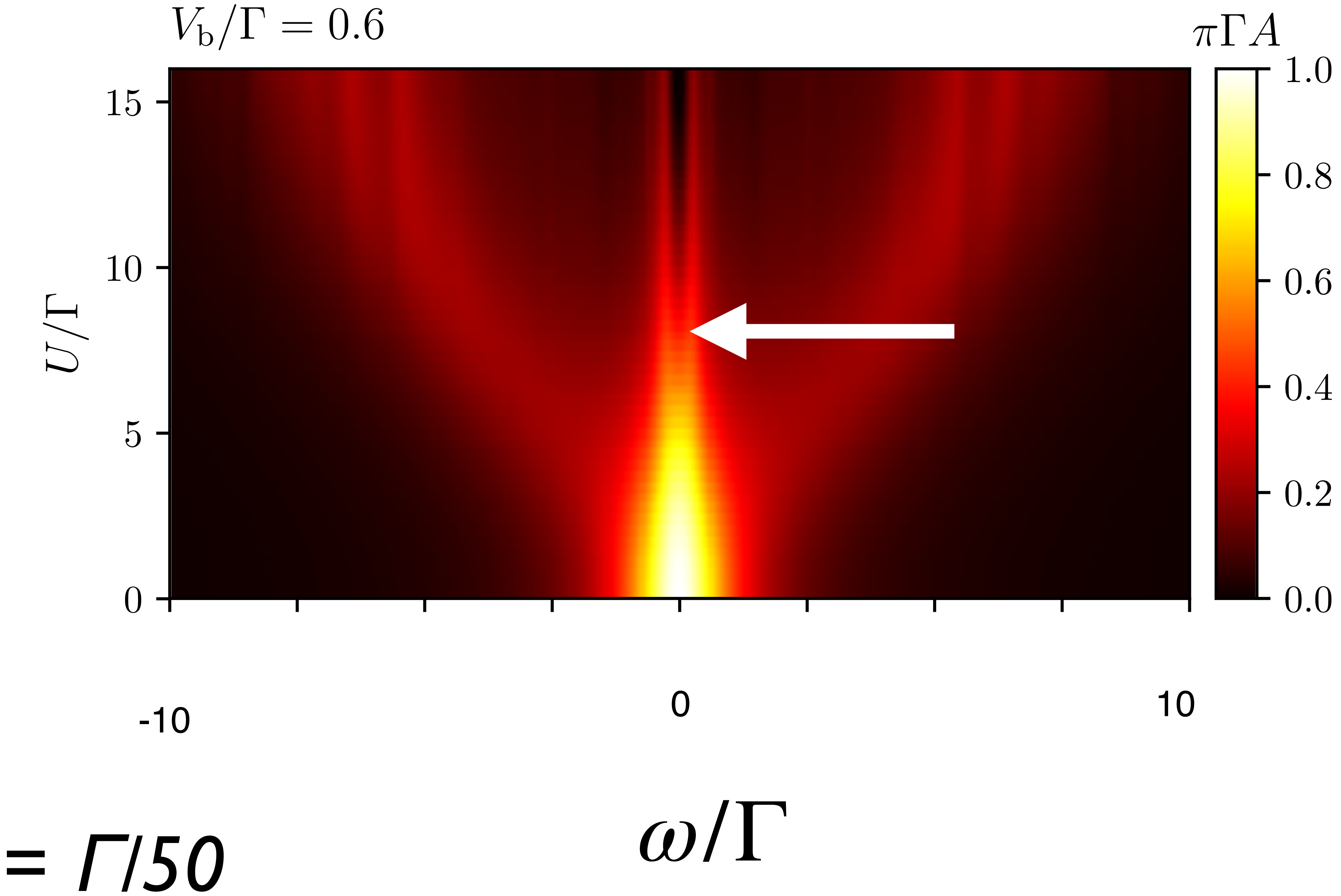
- Change of variable W(U), with W(0) = 0

$$Q = \sum_{n\geq 0} Q_n U^n = \sum_{p\geq 0} \bar{Q}_p W^p$$

Converges at W_0

Out of equilibrium. Steady state

Kondo resonance

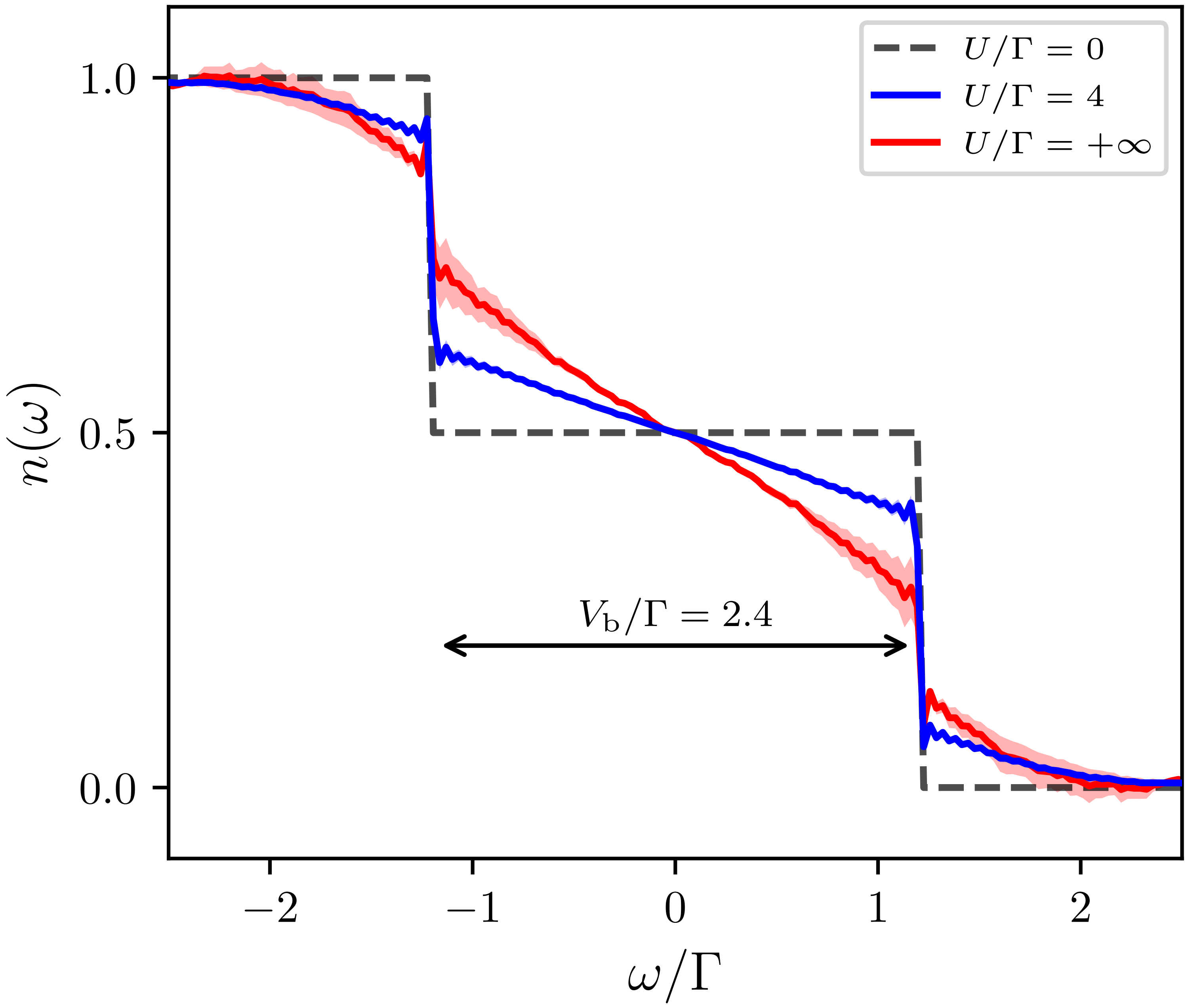


T = Γ/50

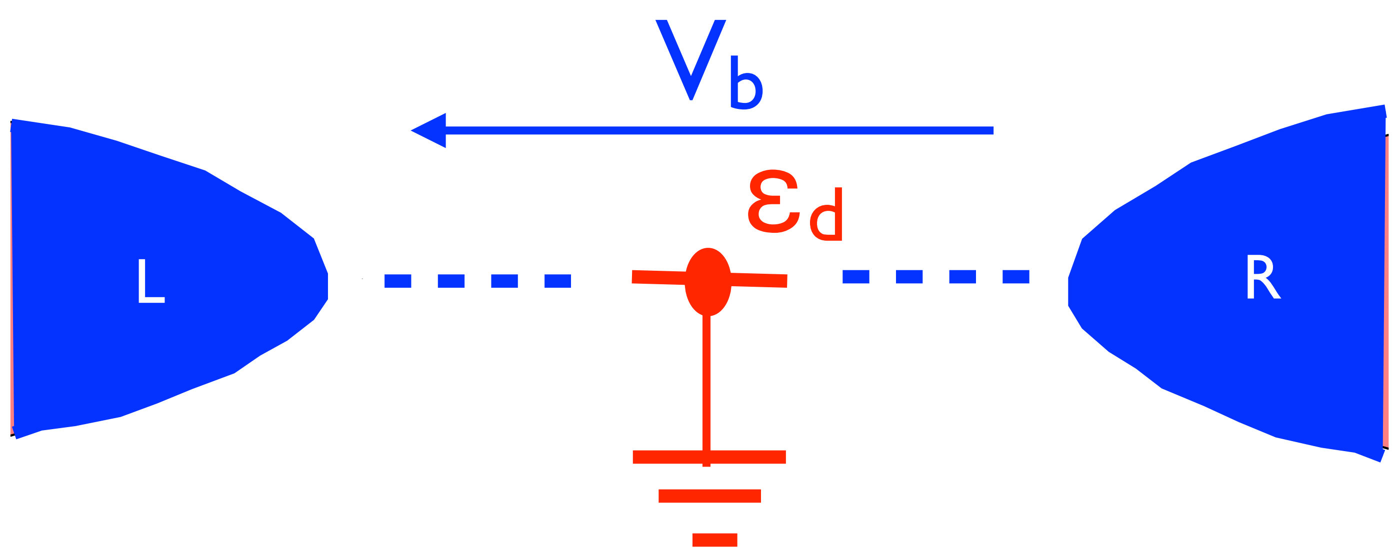
Dot non-thermal distribution function

at $T = 0$ with voltage V_b

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



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



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

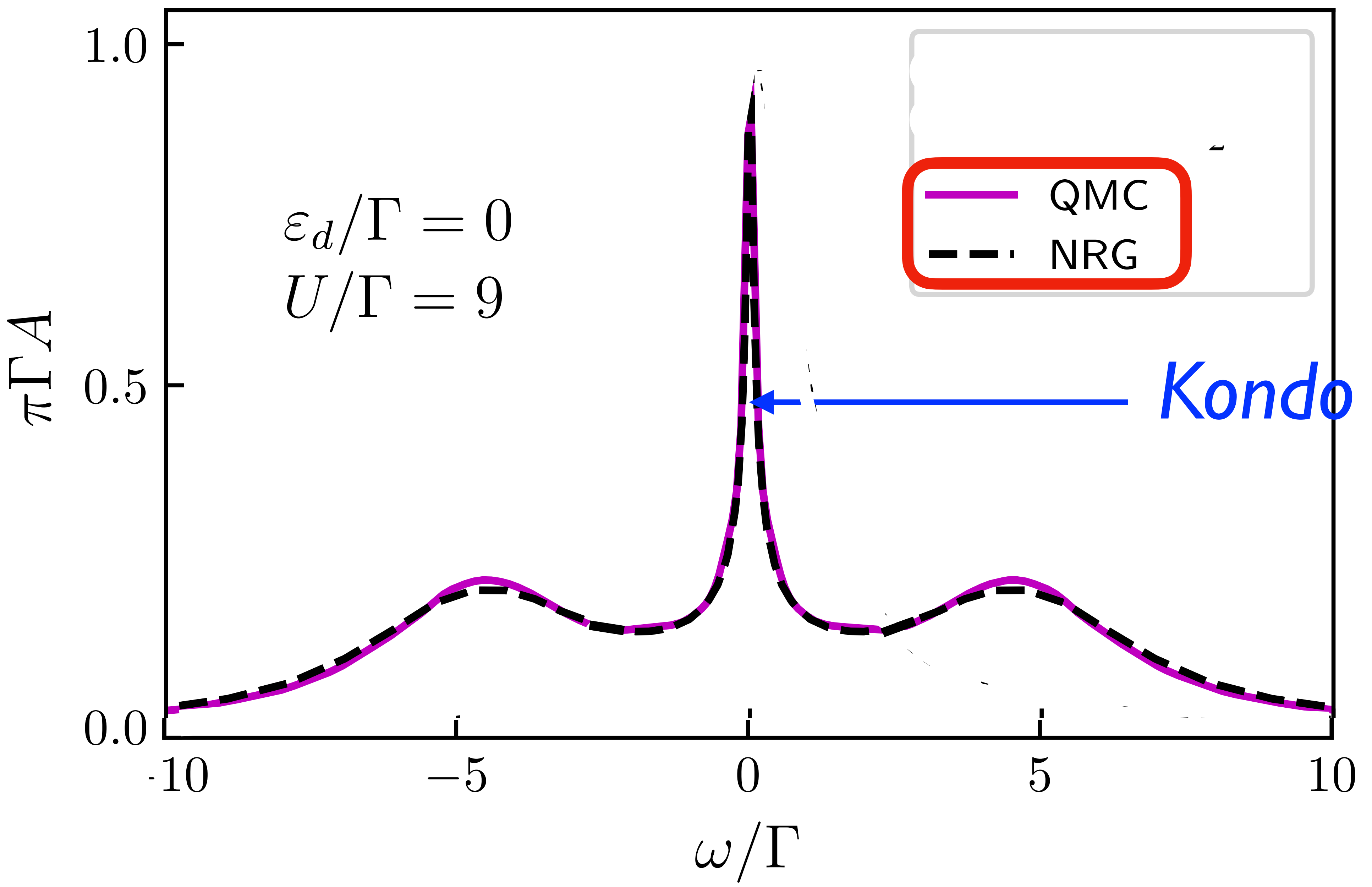
Kondo effect in equilibrium

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

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

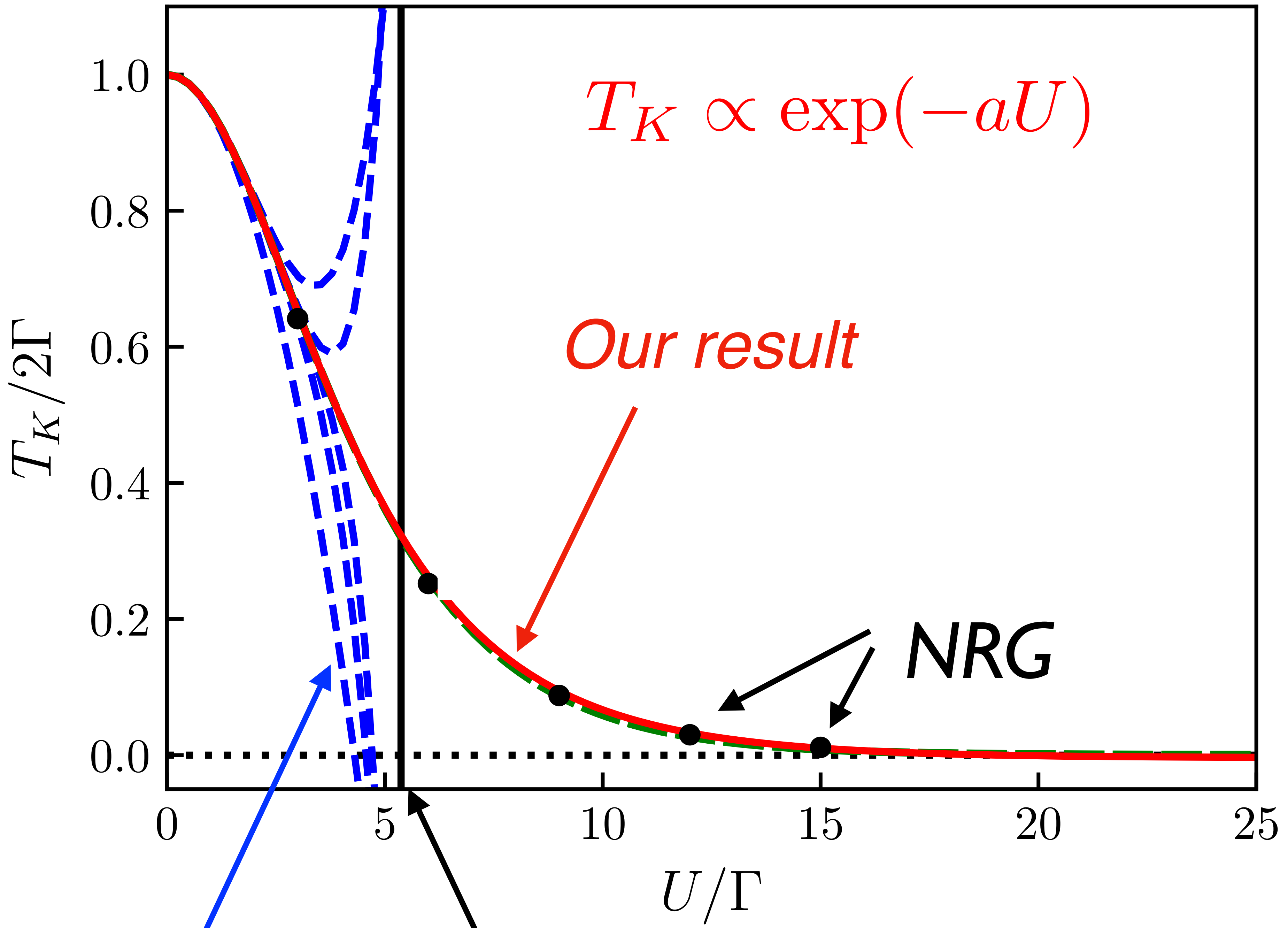
Spectral function of the dot

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



Kondo resonance

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



$T_K \propto \exp(-aU)$

Our result

NRG

Truncated sums of the series

Convergence radius