Title: Tensor networks for real materials

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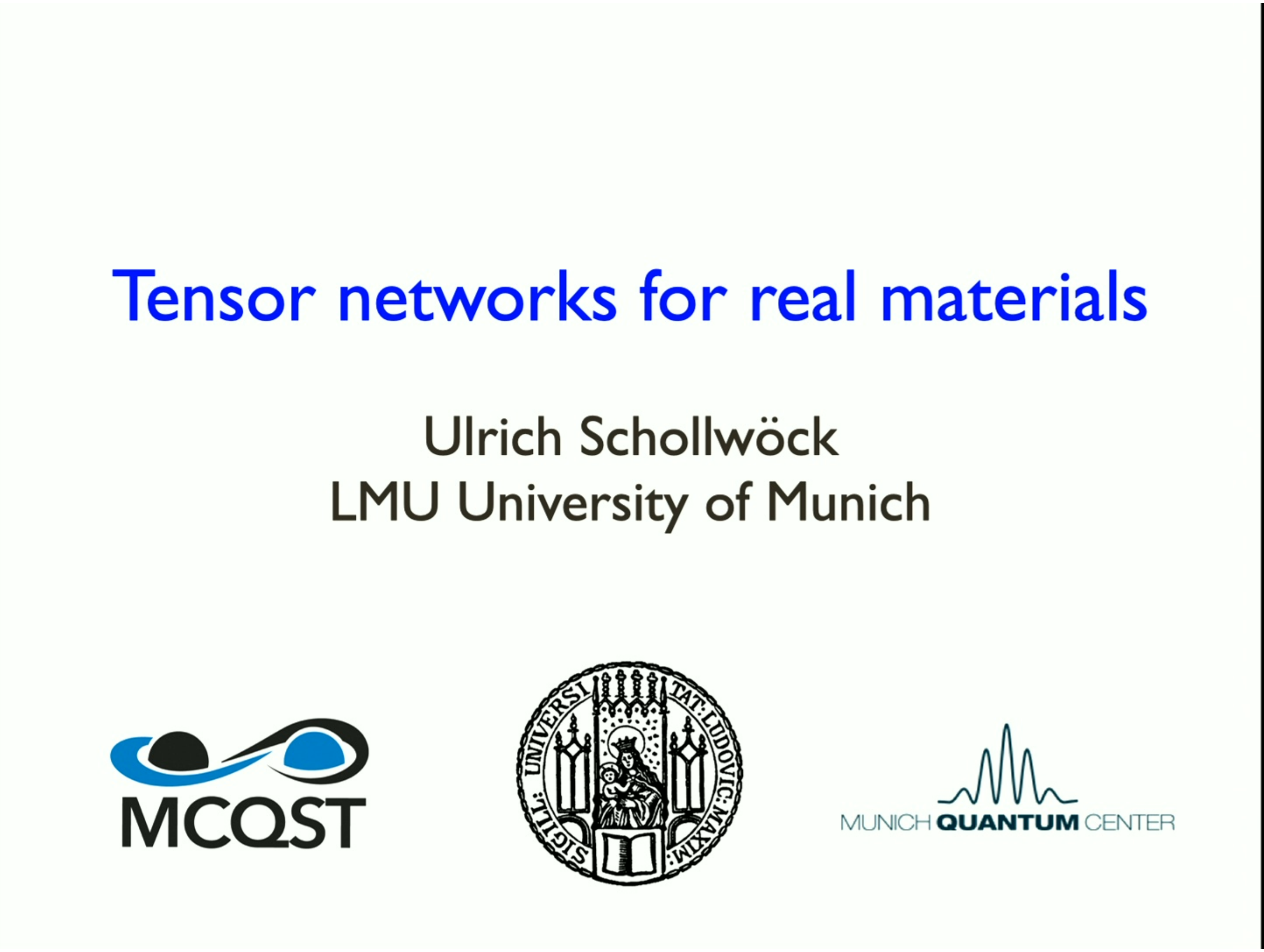
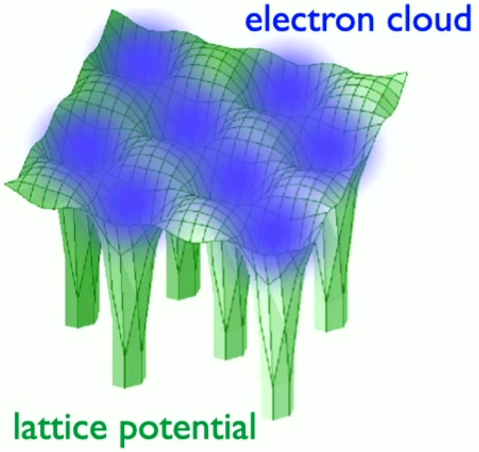


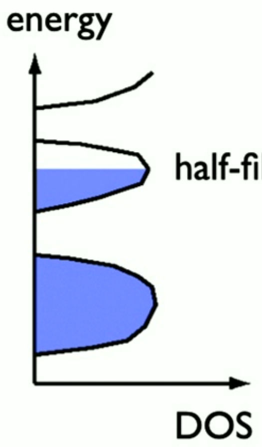
Tensor networks for real materials

Ulrich Schollwöck
LMU University of Munich

many-body problem of solid state I

- **scenario I**
  valence electrons well delocalized
  interactions well screened





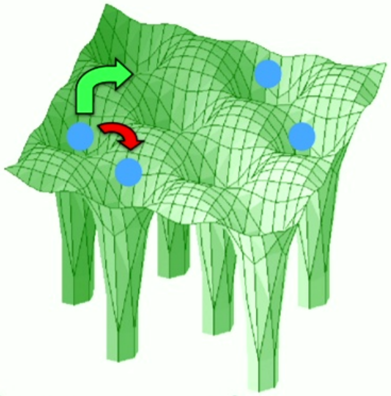
conductor

- many metals, semiconductors: single-electron picture OK

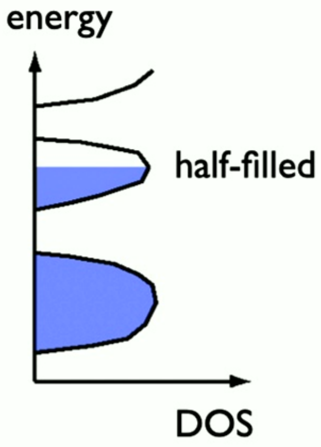
density functional theory (DFT)

many-body problem of solid state II

- **scenario II**
  valence electrons tightly bound
  strong local interactions



lattice potential



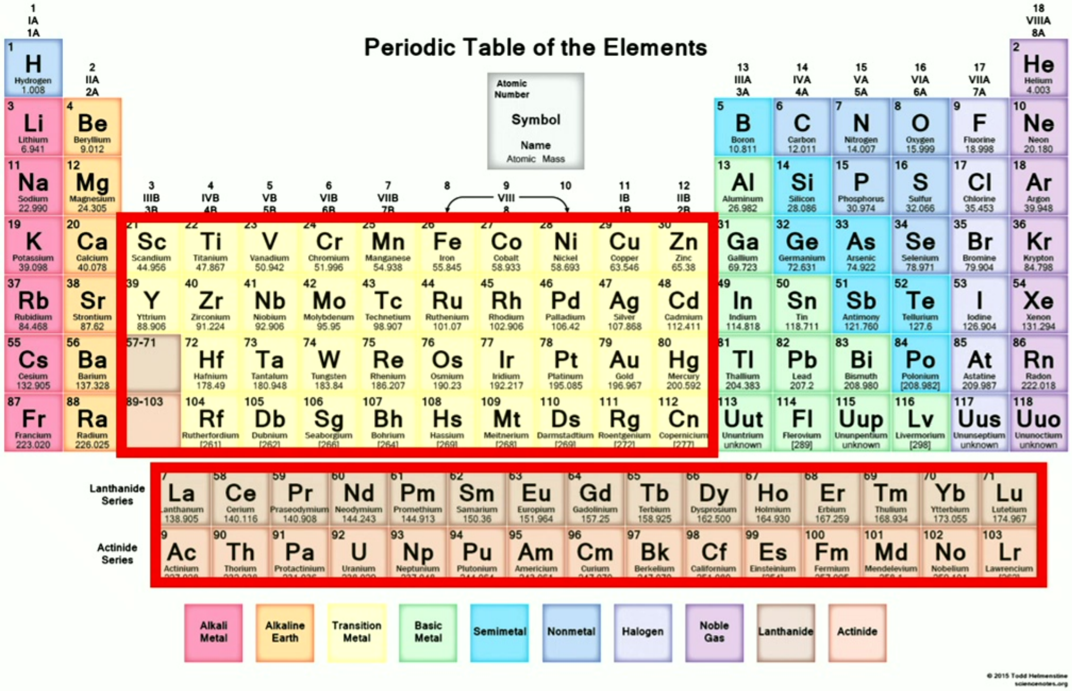
insulator

eg. high-Tc
parent compounds

- many particle picture: **strongly correlated materials**

model Hamiltonian methods - realism ??

transition metal oxides and rare earths



- belated filling of the *d*- and *f*-shells
  valence electrons quite tightly bound
  strong correlations: single-particle picture fails

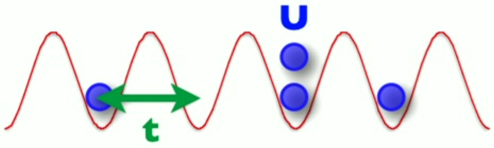
model Hamiltonians …

- typical model Hamiltonian: Hubbard model (1964)

  single band version:

$$\boxed{H = -t \sum_{\langle i,j\rangle;\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + h.c. + U \sum_{i} n_{i\uparrow} n_{i\downarrow}}$$

Wannier basis   kinetic energy   Coulomb energy



crystal lattice: sit only at fixed positions („sites“)

kinetic energy: hop only from one site to the next

charge repulsion: only repel on same site

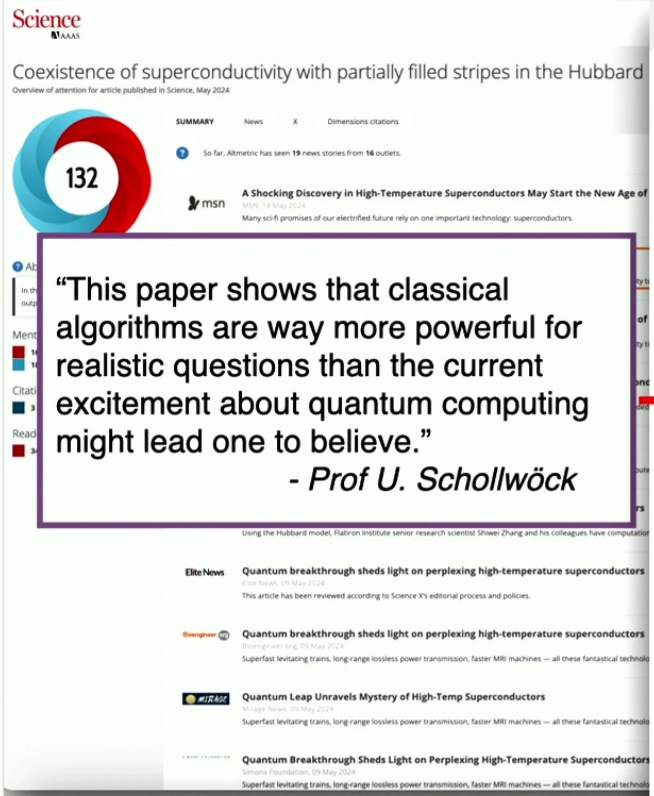
- most simple cartoon version of a correlated problem

  high-Tc model? no! need more (Qin *et al.*, PRX (20); Xu *et al.* (24))

- no exact solution except for *d*=1 after 50 years!

Xu, Chung, Qin, US, White, Zhang: Science **384**, 637 (2024)

Superconductivity and Beyond ?



Science AAAS

Coexistence of superconductivity with partially filled stripes in the Hubbard

Overview of attention for article published in Science, May 2024

So far, Altmetric has seen **19** news stories from **16** outlets.

A Shocking Discovery in High-Temperature Superconductors May Start the New Age of
MSN, 14 May 2024
Many sci-fi promises of our electrified future rely on one important technology: superconductors.

Using the Hubbard model, Flatiron Institute senior research scientist Shiwei Zhang and his colleagues have computation

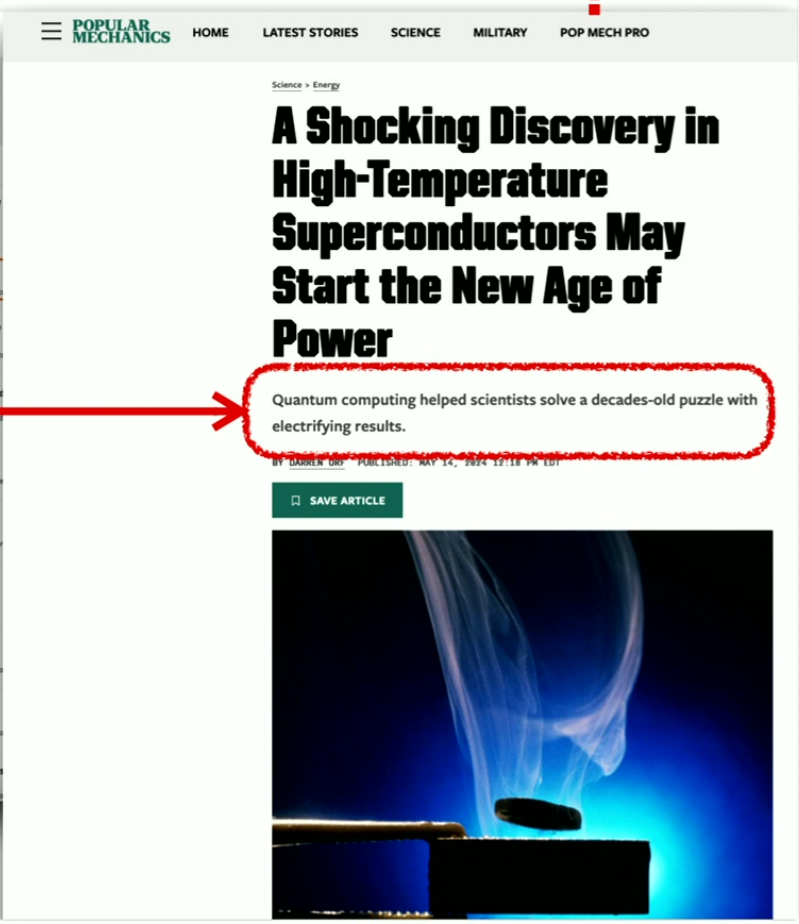
Quantum breakthrough sheds light on perplexing high-temperature superconductors
Elite News, 09 May 2024
This article has been reviewed according to Science X's editorial process and policies.

Quantum breakthrough sheds light on perplexing high-temperature superconductors
Bioengineer.org, 09 May 2024
Superfast levitating trains, long-range lossless power transmission, faster MRI machines — all these fantastical technolo

Quantum Leap Unravels Mystery of High-Temp Superconductors
Mirage News, 09 May 2024
Superfast levitating trains, long-range lossless power transmission, faster MRI machines — all these fantastical technolo

Quantum Breakthrough Sheds Light on Perplexing High-Temperature Superconductors
Simons Foundation, 09 May 2024
Superfast levitating trains, long-range lossless power transmission, faster MRI machines — all these fantastical technolo

> "This paper shows that classical algorithms are way more powerful for realistic questions than the current excitement about quantum computing might lead one to believe."
> *- Prof U. Schollwöck*



Science > Energy

A Shocking Discovery in High-Temperature Superconductors May Start the New Age of Power

Quantum computing helped scientists solve a decades-old puzzle with electrifying results.

BY DARREN ORF PUBLISHED: MAY 14, 2024 12:18 PM EDT

MPS meet DMFT

goal: become more realistic by teaming up with other method!


Claudius Hubig


Nils Linden


Martin Grundner


Max Bramberger

Olivier Parcollet, Antoine Georges, *CCQ/CEA Saclay/Polytechnique*
Uli Schollwöck, *LMU Munich/CCQ (visitor)*
Manuel Zingl, Alex Hampel, Fabian Kugler, Andy Millis, *CCQ*
Jernej Mravlje, *Josef Stefan Institute, Ljubljana*
Benjamin Bacq-Labreuil, Benjamin Lenz, Silke Biermann, *Paris*

Wolf et al, PRB 90, 115124 (2014)

Wolf et al, PRX 5, 041032 (2015)

Linden et al, PRB 101, 041101 (R) (2020)

Karp et al, PRL 125, 166401 (2020)

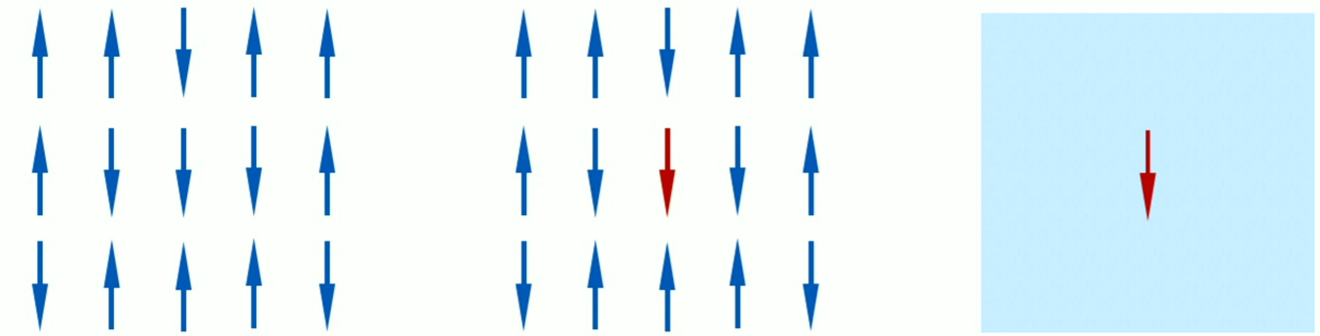
Bramberger et al, PRB 103, 165133 (2021)

Bramberger et al., SciPost Phys. (2023)

Grundner et al., PRB 109, 155124 (2024)

Grundner et al., 2409.17268 (2024)

mean-field theory

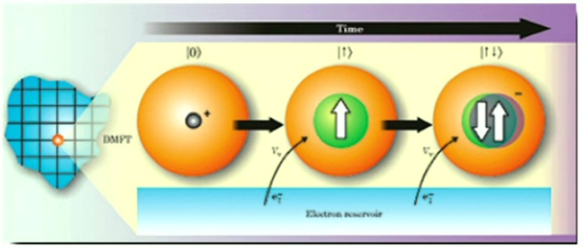


spins interact & fluctuate   pick 1: lose spatial dependence   in effective field of others

- Weiss mean-field theory:
  replace fluctuating environment by static field
- self-consistency condition: $\langle S \rangle = \tanh \beta J \langle S \rangle$
  - spin has magnetization it would have in effective field created by it
- magnetization $\langle S \rangle$: order parameter of phase transition

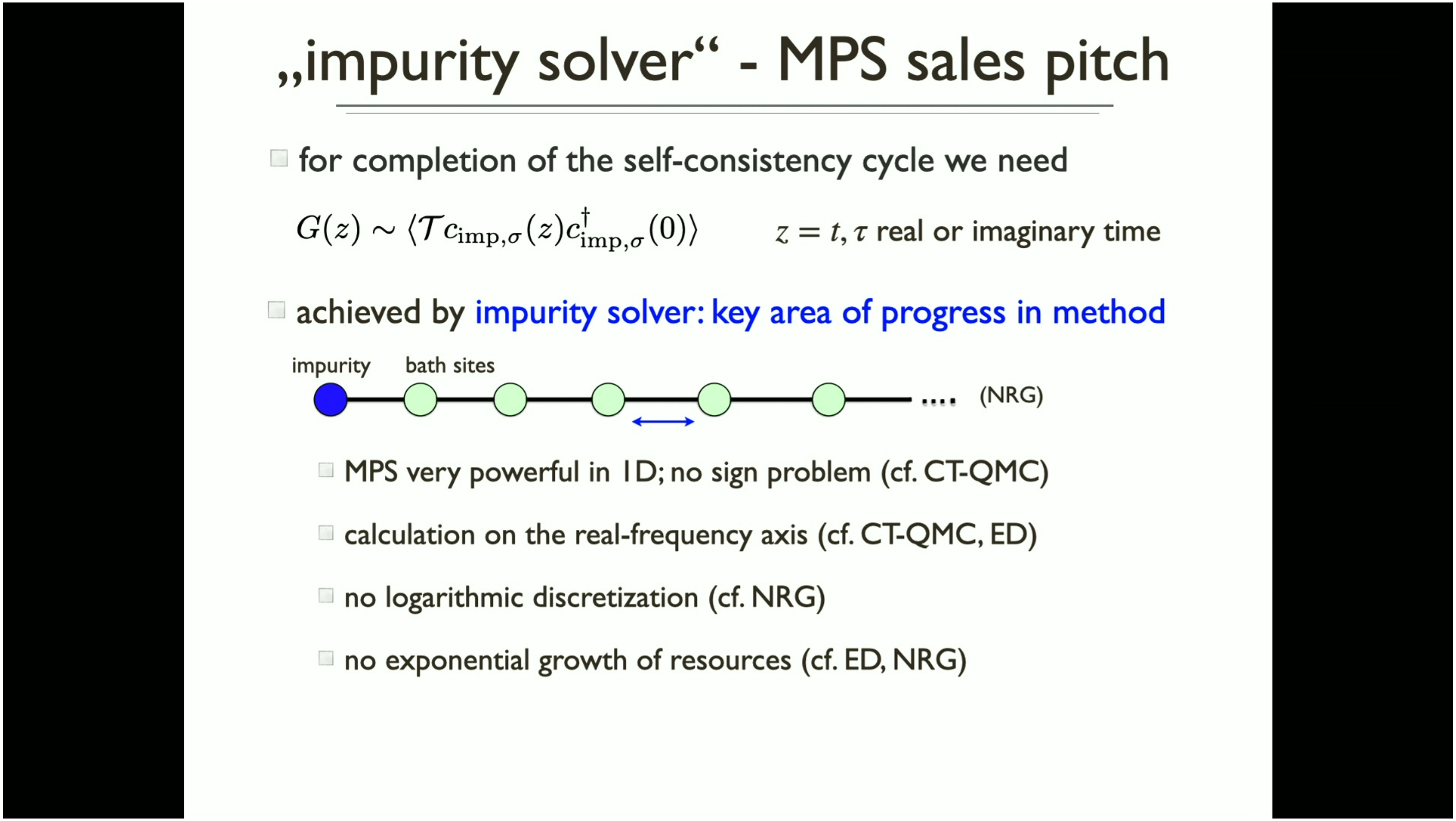
DMFT

- dynamical mean field theory (DMFT)
  - interacting model → interacting „impurity“ in non-interacting effective bath



  - impurity dynamically exchanges electrons with bath
  - dynamical self-consistency: local lattice GF/SE = impurity GF/SE
- exact in the limit of infinite coordination number (dimension)
- more realism by
  - multiple bands
  - cluster methods (CDMFT, DCA)
  - combination with DFT

Georges, Kotliar, PRB (1992)
Georges *et al.*, RMP (1996)
Kotliar *et al.*, RMP (2006)
(…)



„impurity solver“ - MPS sales pitch

- for completion of the self-consistency cycle we need

$$G(z) \sim \langle \mathcal{T} c_{\mathrm{imp},\sigma}(z) c^{\dagger}_{\mathrm{imp},\sigma}(0) \rangle \qquad z = t, \tau \text{ real or imaginary time}$$

- achieved by impurity solver: key area of progress in method

impurity
bath sites
(NRG)

- MPS very powerful in 1D; no sign problem (cf. CT-QMC)
- calculation on the real-frequency axis (cf. CT-QMC, ED)
- no logarithmic discretization (cf. NRG)
- no exponential growth of resources (cf. ED, NRG)

MPS meets DMFT: history

- 1 orbital DMFT: around 2006
- 2 orbital DMFT/DCA: 2014

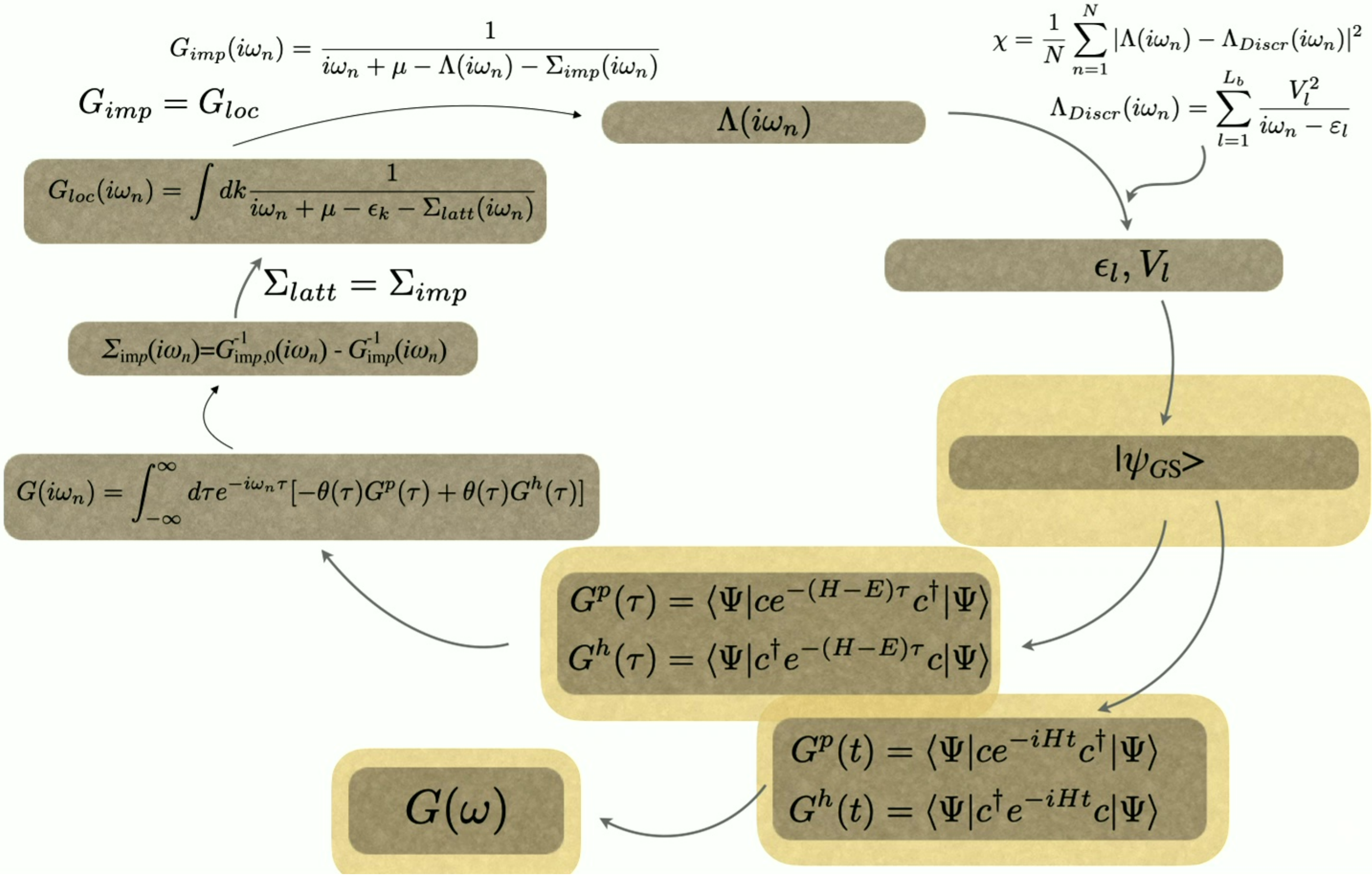
Wolf, McCulloch, Parcollet, US, PRB (2014)
Ganahl *et al*, PRB (2014), PRB (2015)

- various axes of development after
- we: switch to imaginary axis (cf. ED):
  - much smaller bath sizes
  - no entanglement growth in time evolution
  - much larger number of orbitals
  - analytic continuation of spectral function

Wolf, Go, McCulloch, Millis, US,
PRX 5, 041032 (2015)

- convincing results for **6 orbitals** (simplified band structure)
- what about realistic band structures?

imaginary-time DMFT-MPS



$$G_{imp}(i\omega_n) = \frac{1}{i\omega_n + \mu - \Lambda(i\omega_n) - \Sigma_{imp}(i\omega_n)}$$

$$G_{imp} = G_{loc}$$

$$\Lambda(i\omega_n)$$

$$\chi = \frac{1}{N}\sum_{n=1}^{N} |\Lambda(i\omega_n) - \Lambda_{Discr}(i\omega_n)|^2$$

$$\Lambda_{Discr}(i\omega_n) = \sum_{l=1}^{L_b} \frac{V_l^2}{i\omega_n - \varepsilon_l}$$

$$G_{loc}(i\omega_n) = \int dk \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_{latt}(i\omega_n)}$$

$$\epsilon_l, V_l$$

$$\Sigma_{latt} = \Sigma_{imp}$$

$$\Sigma_{\text{imp}}(i\omega_n) = G^{-1}_{\text{imp},0}(i\omega_n) - G^{-1}_{\text{imp}}(i\omega_n)$$

$$|\psi_{GS}>$$

$$G(i\omega_n) = \int_{-\infty}^{\infty} d\tau e^{-i\omega_n\tau}[-\theta(\tau)G^p(\tau) + \theta(\tau)G^h(\tau)]$$

$$G^p(\tau) = \langle\Psi|ce^{-(H-E)\tau}c^\dagger|\Psi\rangle$$

$$G^h(\tau) = \langle\Psi|c^\dagger e^{-(H-E)\tau}c|\Psi\rangle$$

$$G^p(t) = \langle\Psi|ce^{-iHt}c^\dagger|\Psi\rangle$$

$$G^h(t) = \langle\Psi|c^\dagger e^{-iHt}c|\Psi\rangle$$

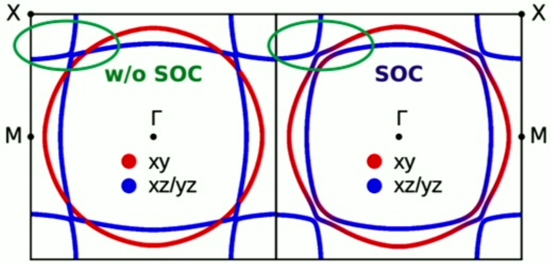
$$G(\omega)$$

Sr_2RuO_4 - a Hund's metal with spin-orbit coupling

or: back to the drawing board …

Sr_2RuO_4

☐ band structure from DFT



☐ interaction: 3 band-Hubbard-Kanamori (t_{2g})

$$\hat{H}_{\text{int}} = (U-3J)\frac{\hat{N}^2-\hat{N}}{2} - 2J\hat{\mathbf{S}}^2 - \frac{1}{2}J\hat{\mathbf{L}}^2 + \frac{5}{2}J\hat{N}$$

U=2.3 eV
J=0.4 eV
λ=0.1 eV

☐ spin-orbit coupling

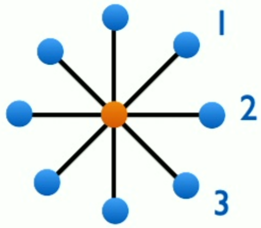
DFT: topology changed at degeneracy

$$\hat{H}_{\text{SOC}} = \frac{\lambda}{2}\sum_{mm'}\sum_{\sigma\sigma'}\hat{d}^{\dagger}_{m\sigma}\left(\mathbf{l}_{mm'}\cdot\boldsymbol{\sigma}_{\sigma\sigma'}\right)\hat{d}_{m'\sigma'}$$

how do I map a bath to 1D MPS?

„natural“ DMFT bath geometry

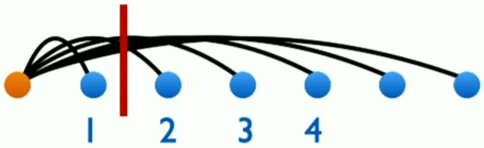
Wolf, McCulloch, Schollwöck, PRB 90, 235131 (2014)



impurity

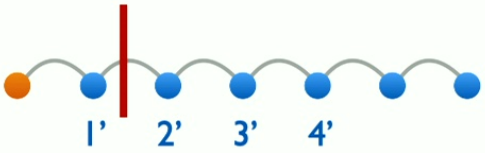
non-interacting bath sites

approach A: „star“ geometry



- ☐ long-ranged hopping
- ☐ strongly entangled (?)

approach B: chain geometry obtained by tridiagonalization



- ☐ required in NRG (separation of energy scales)
- ☐ weakly entangled (?) - good for MPS

how do I map a bath to 1D MPS?

„natural“ DMFT bath geometry

Wolf, McCulloch, Schollwöck, PRB 90, 235131 (2014)

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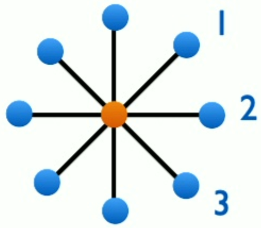
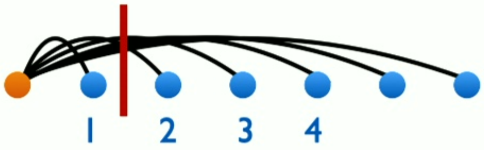


approach A: „star“ geometry



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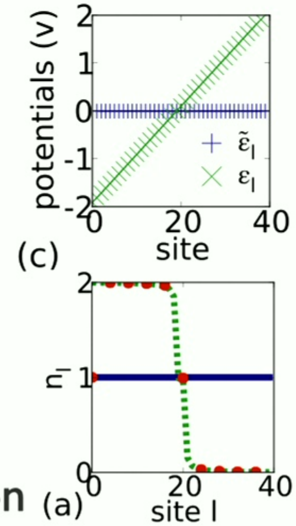
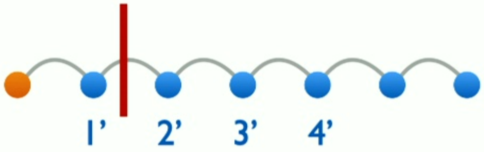


approach B: chain geometry obtained by tridiagonalization



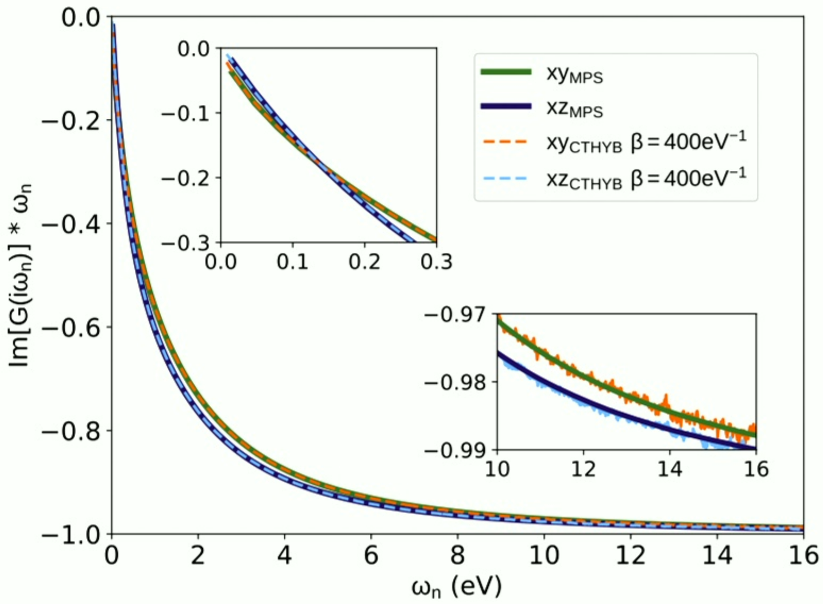
- ☐ required in NRG (separation of energy scales)
- ☐ weakly entangled (?) - good for MPS

no!

benchmarking: CTQMC vs MPS

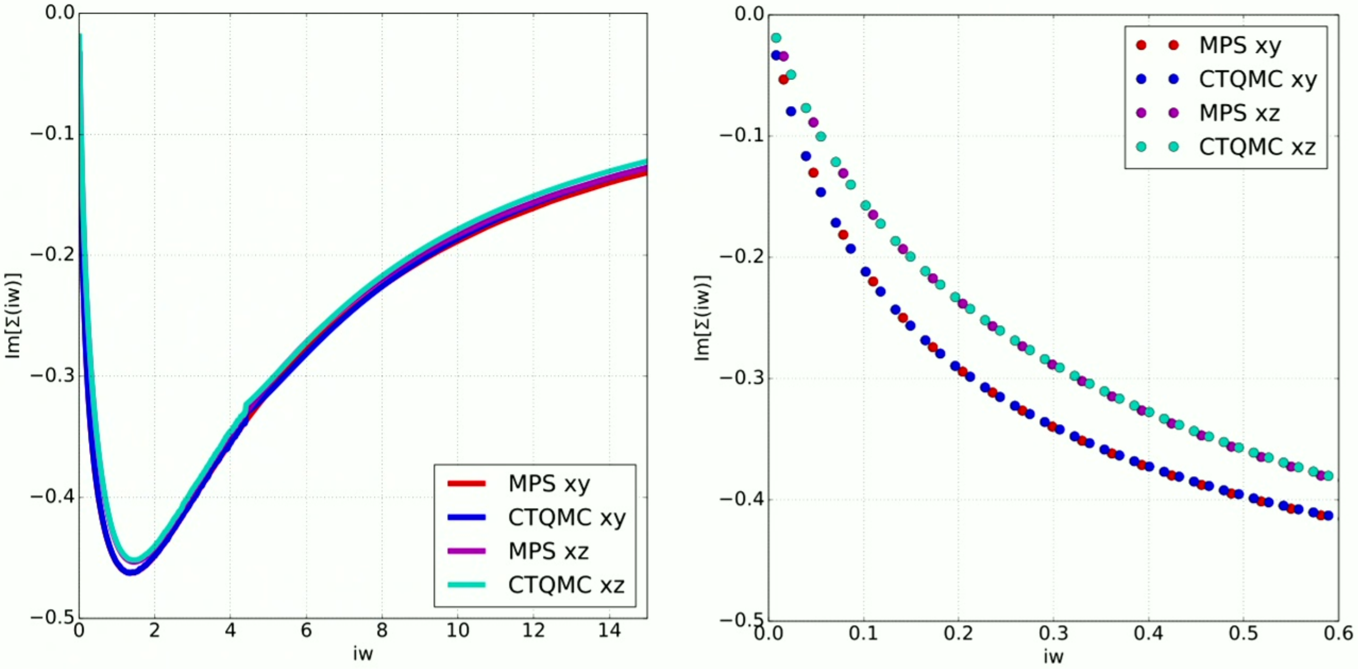
- $\tau < 4$: Krylov $\Delta\tau = 0.0005$ from timestep $\Delta\tau = 0.1$
- $\tau > 4$: 2TDVP with timestep $\Delta\tau = 0.1$
- don't use Trotter

short-time
time-stepping
issues



- CTQMC/MPS perfectly on top!
- no fit/noise in MPS

self-energy: effect of correlations



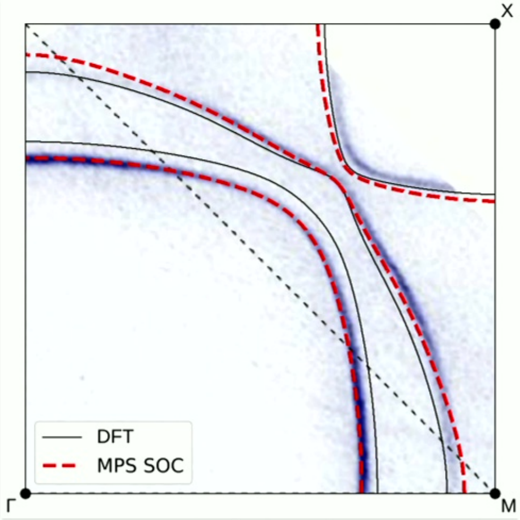
- overall agreement very good
- same small-frequency behaviour (extrapolates to zero)

SOC: comparison to ARPES

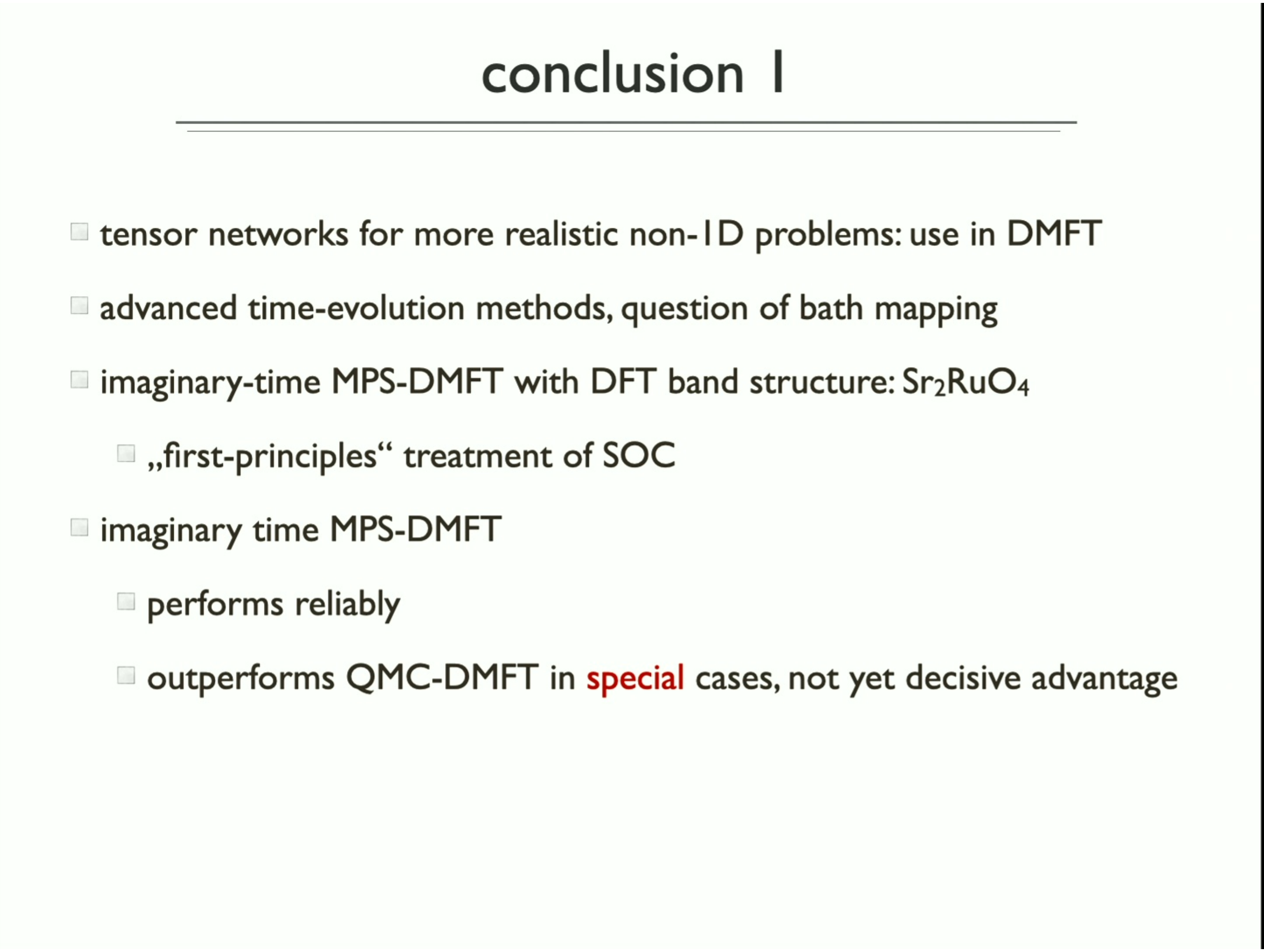
- fit-free comparison to ARPES (Tamai et al, PRX (2019))

  [greyscale: ARPES signal]

- interaction shifts Fermi surface on experimental positions



- more three-band work with SOC:
  - Sr_2MoO_4 Karp et al, PRL 125, 166401 (2020)
  - $BaOsO_3$ Bramberger et al, PRB 103, 165133 (2021)



conclusion I

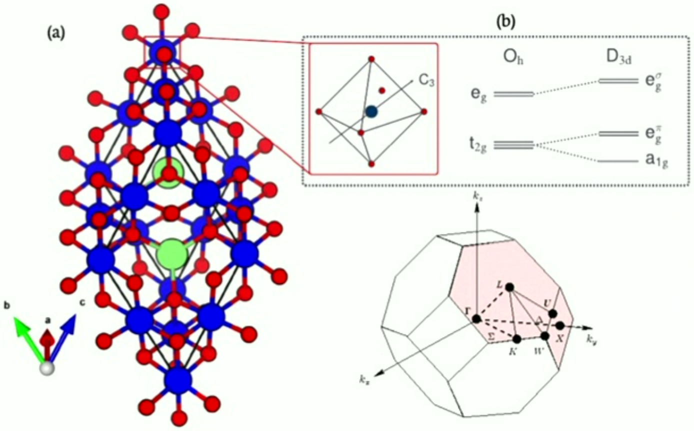
- tensor networks for more realistic non-1D problems: use in DMFT
- advanced time-evolution methods, question of bath mapping
- imaginary-time MPS-DMFT with DFT band structure: Sr_2RuO_4
  - „first-principles“ treatment of SOC
- imaginary time MPS-DMFT
  - performs reliably
  - outperforms QMC-DMFT in special cases, not yet decisive advantage

LiV_2O_4: „Hund-assisted orbital-selective Mottness“

M. Grundner, F. Kugler, O. Parcollet, U. Schollwöck, A. Georges, A. Hampel
(2409.17268)

LiV_2O_4: basics

- local symmetry splits 5 *d*-orbitals of V:
  - 3 low-lying t_{2g} orbitals, 2 e_g
  - t_{2g} orbitals split in 2 e^{π}_g, 1 a_{1g}
- 1.5 electrons per V
- geometric frustration
  (no magnetic order)
- Fermi liquid scale ($\rho \propto T^2$) well below 10 K
- large mass enhancement below 25 K: $m^*/m \sim 25$



LiV_2O_4

(Kondo PRL 1997)

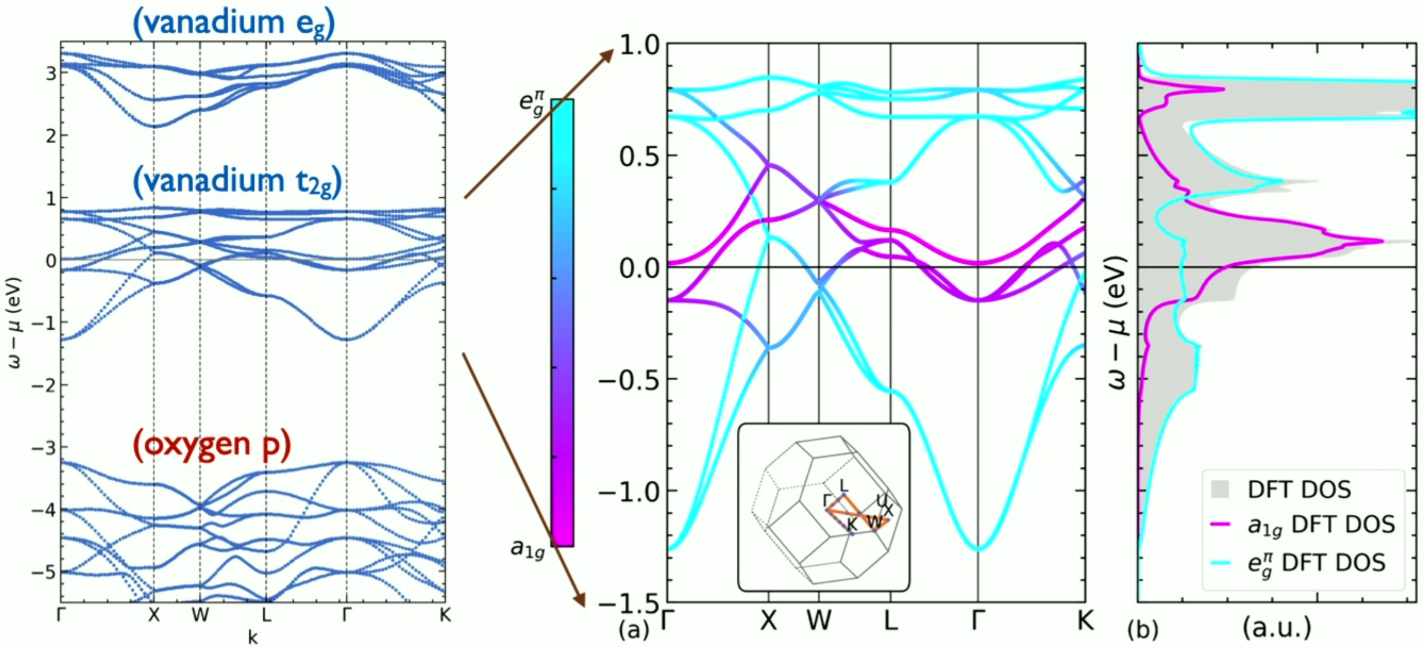
intensively studied since late 90es
(sort of) „heavy fermion physics" in a transition metal oxide

where does this come from?

- standard explanation of heavy fermions in rare earths (localized *f*-electrons meet itinerant *d*-electrons) cannot work
- adaptation: *f*-electrons → a_{1g} electrons
  d-electrons → e^{π}_{g} electrons (Anisimov *et al* PRL 1999)
- Kondo-like explanation does not work (Arita *et al* PRL 2007)
  (FM Hund's coupling dominates AFM Kondo, exp. details)

  instead: (Arita PRL 2007)
  a_{1g} band lightly doped ($n \approx 0.98$)
  e^{π}_{g} bands bystanders
  strong mass renormalization due to proximity to Mott transition
- (…)
- common problem: temperature! 11,000 K vs. 10 K, achieve 300 K …

DFT band structure



- zoom in; contribution of t_{2g} orbitals

local interactions: DFT+DMFT

- Hubbard-Kanamori model (3-band Hubb. with Hund's coupling *J*)

$U = 3.94\text{eV}$

$U' = 2.83\text{eV}$

$J = 0.56\text{eV}$

$$\begin{aligned}\hat{H}_K = {} & U \sum_{m} \hat{n}_{m\uparrow}\hat{n}_{m\downarrow} + U' \sum_{m\neq m'} \hat{n}_{m\uparrow}\hat{n}_{m'\downarrow} \\ & + (U'-J) \sum_{m<m',\sigma} \hat{n}_{m\sigma}\hat{n}_{m'\sigma} - J \sum_{m\neq m'} \hat{d}^{\dagger}_{m\uparrow}\hat{d}_{m\downarrow}\hat{d}^{\dagger}_{m'\downarrow}\hat{d}_{m'\uparrow} \\ & + J \sum_{m\neq m'} \hat{d}^{\dagger}_{m\uparrow}\hat{d}^{\dagger}_{m\downarrow}\hat{d}_{m'\downarrow}\hat{d}_{m'\uparrow}, \qquad (25)\end{aligned}$$

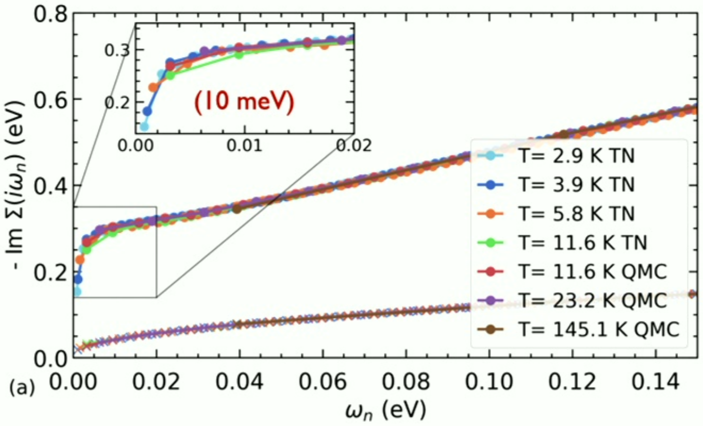
- MPS-DMFT solver extended to finite *T* (purification method)

- QMC-DMFT solver down to as low *T* as possible for benchmark

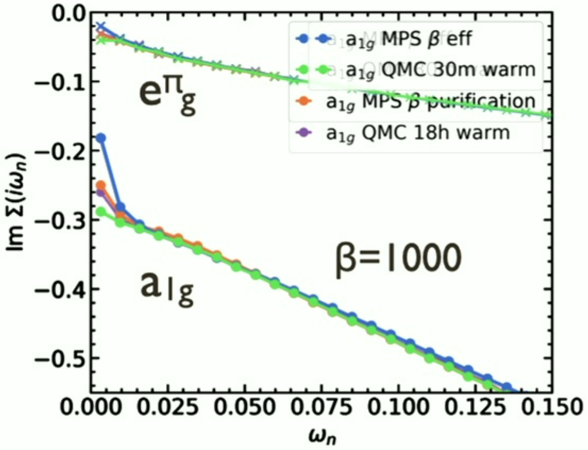
- later: NRG-DMFT solver for lowest *T* and simplified model

Fermi liquid at *extremely low T*

- reach β = 4,000 (2.9 K)
- below approx 10…15 K
  new energy scale / physics
- QMC validates TN



- TN: odd/even effect in bath size
- QMC (rising to challenge):
  - strong warm-up issues
  - 24h warmup at β=1000



consequences of local interactions

☐ DFT occupations

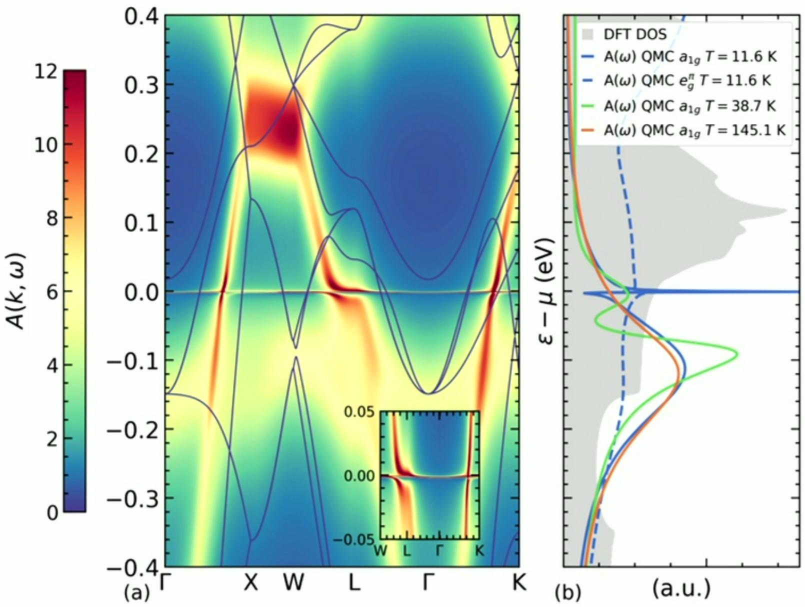
$$n(a_{1g}) = 0.427$$

$$n(e_g^\pi) = 0.537 \quad (\times 2)$$

☐ become in DMFT

$$n(a_{1g}) \approx 0.9$$

$$n(e_g^\pi) \approx 0.3 \quad (\times 2)$$

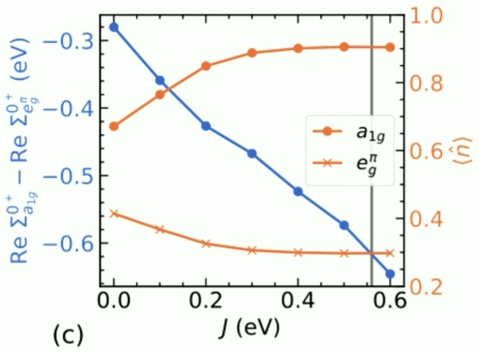


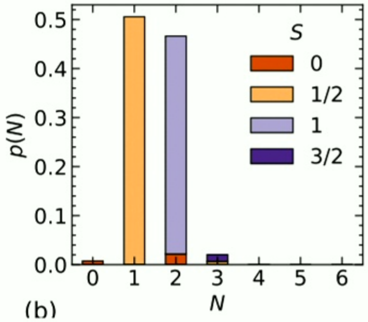
☐ strong peak of DOS at Fermi energy

☐ extremely flat band

what is happening? Hund's coupling!

- effect strongly dependent on **Hund's coupling**



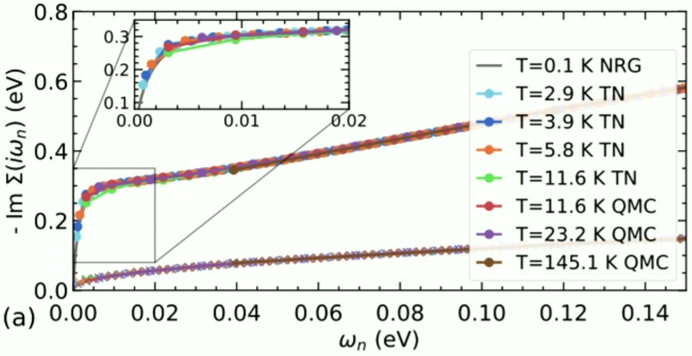


- mechanism (Figs. at T=11.6K)
  - Hund repopulates orbitals
  - Hund inhibits low-energy motion (high spin states) **low-energy flat band**
  - **orbital selective Mott-like physics**
  - robust under a_{1g} doping, J

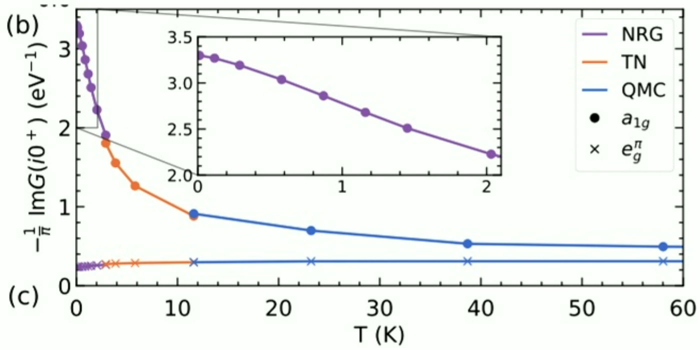
- e^{π}_{g} bands **not just** bystanders

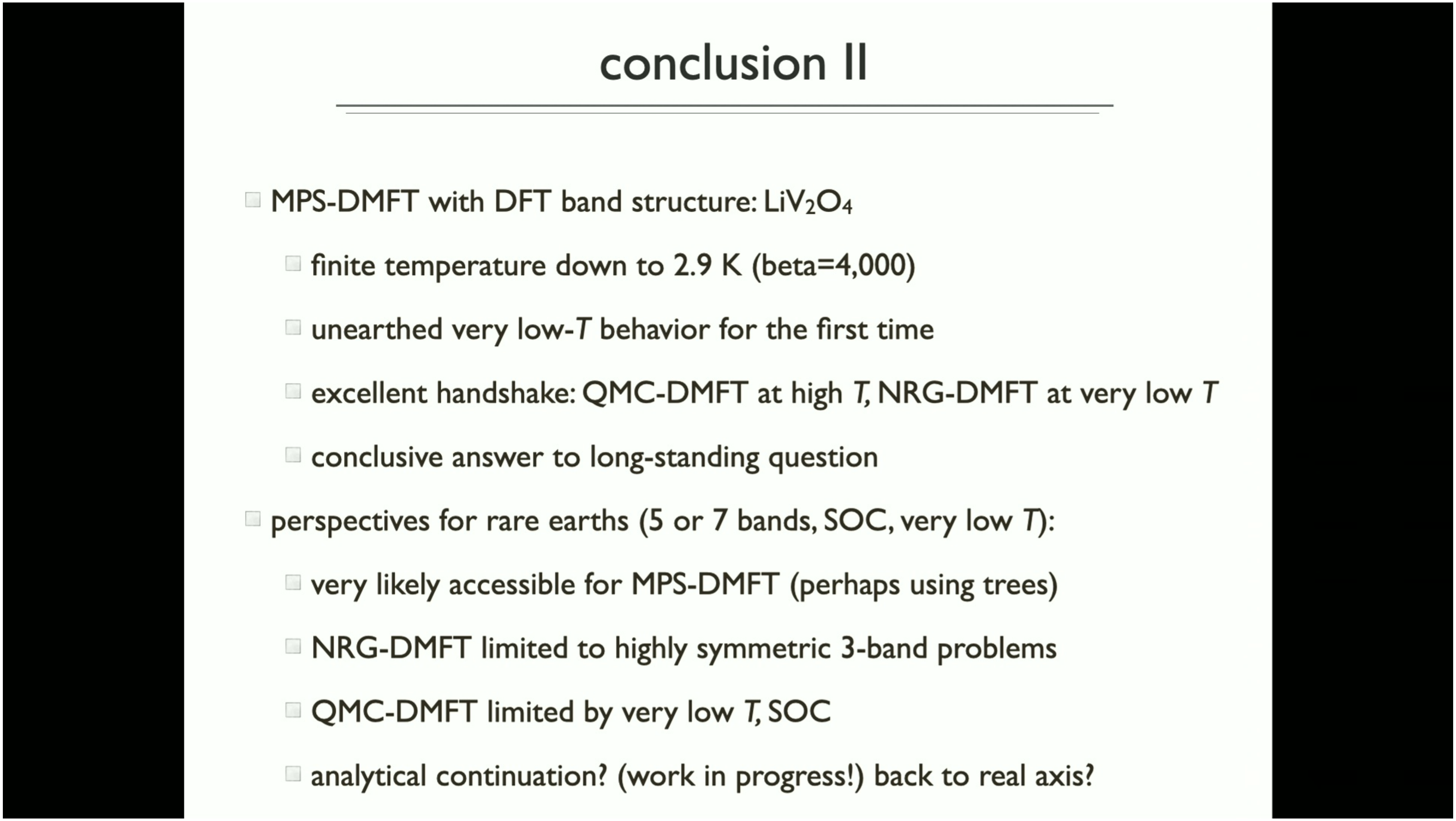
reliability: examples of handshakes

- imaginary part of self-energy (lifetime of quasiparticles)



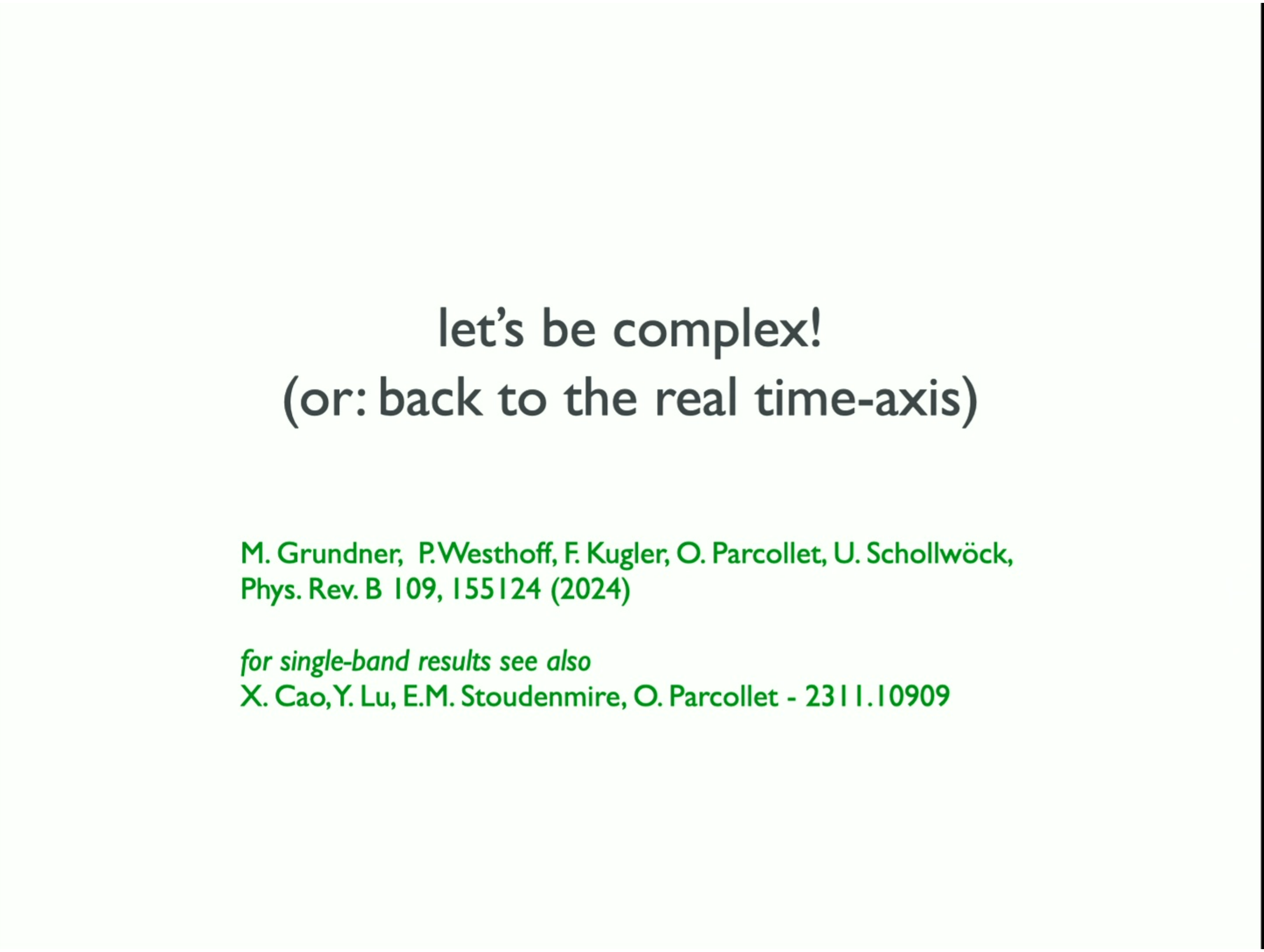
- spectral weight at the Fermi edge





conclusion II

- MPS-DMFT with DFT band structure: LiV_2O_4
  - finite temperature down to 2.9 K (beta=4,000)
  - unearthed very low-*T* behavior for the first time
  - excellent handshake: QMC-DMFT at high *T*, NRG-DMFT at very low *T*
  - conclusive answer to long-standing question
- perspectives for rare earths (5 or 7 bands, SOC, very low *T*):
  - very likely accessible for MPS-DMFT (perhaps using trees)
  - NRG-DMFT limited to highly symmetric 3-band problems
  - QMC-DMFT limited by very low *T*, SOC
  - analytical continuation? (work in progress!) back to real axis?



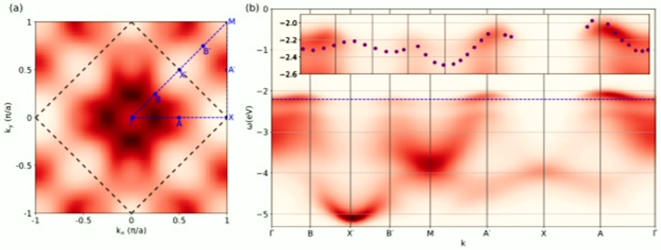
let’s be complex!
(or: back to the real time-axis)

M. Grundner, P. Westhoff, F. Kugler, O. Parcollet, U. Schollwöck,
Phys. Rev. B 109, 155124 (2024)

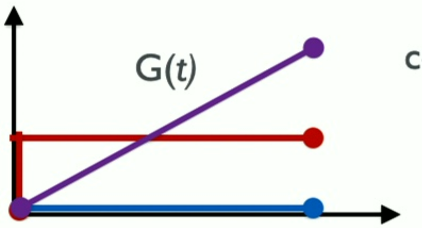
for single-band results see also
X. Cao, Y. Lu, E.M. Stoudenmire, O. Parcollet - 2311.10909

why should we go complex?

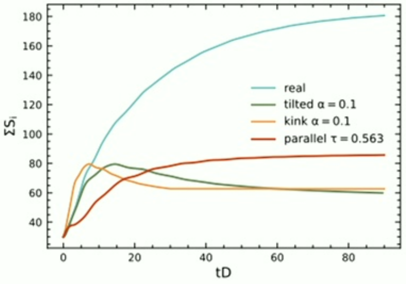
- real-frequency information crucial (scattering, e.g. ARPES, transport)
- require *very low* frequencies
  bandwidth *D* $\approx \mathrm{eV}$
  correlation physics $\approx \mathrm{meV}$
- imaginary-axis calculations:
  - AC difficult, low frequencies bad!
- real-time calculation:
  - limited reach in *t* limits resolution



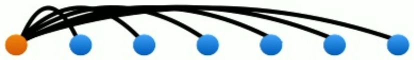
M. Bramberger *et al*, SciPost (2023)



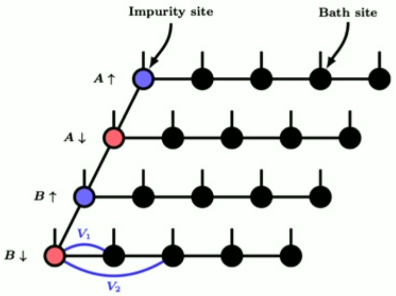
complex *t*



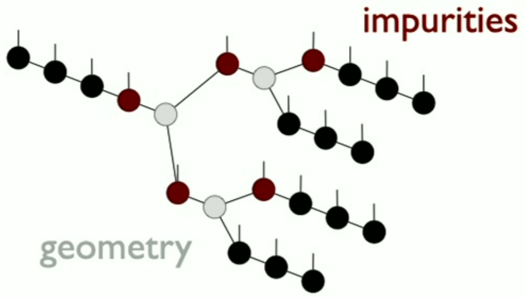
multi-band: which tensor network?



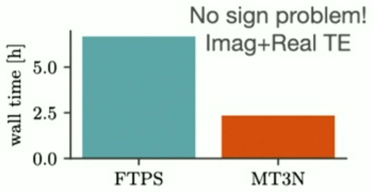
what happens to MPS (in star geometry) when having multiple impurities?



fork tensor network
(Bauernfeind et al. 2018)
- fat four-leg tensors!

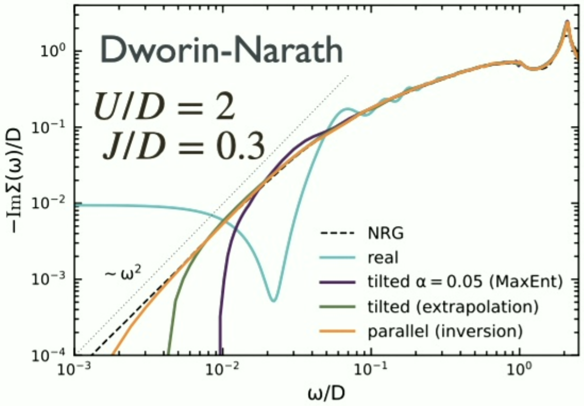


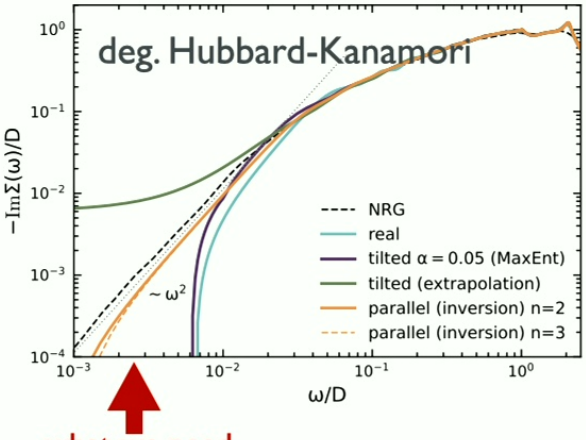
three-legged tensor network
separate physics & geometry
(Gunst et al. 2018)
+ only three-leg tensors!



Benchmarks for $SrMnO_3$:
Speed up by factor of three!

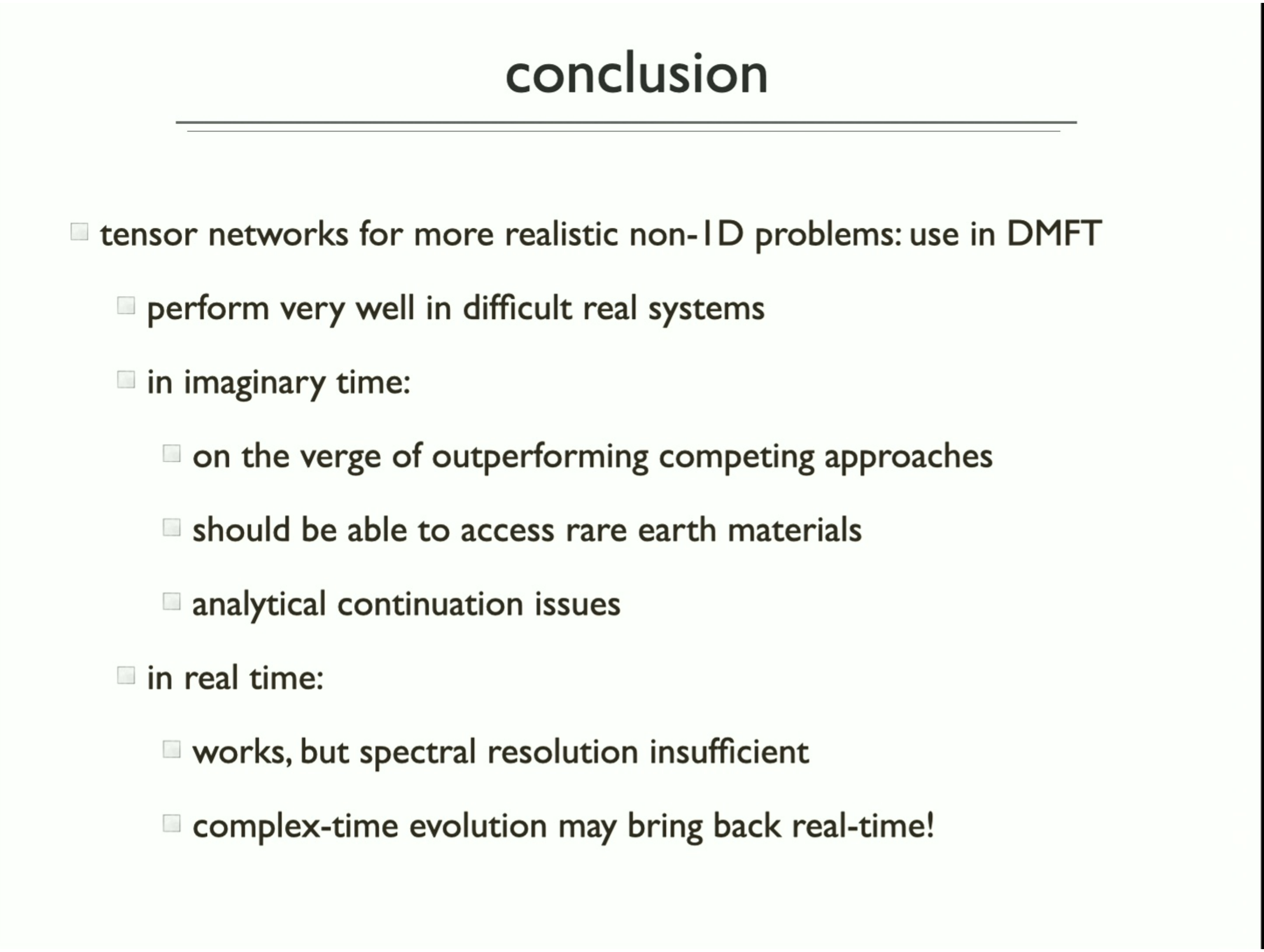
self-energy: three-band models





what we need

- Dworin-Narath:
  - excellent agreement down to very low frequencies
  - remaining difference: Dyson equation!
- deg. Hubbard-Kanamori:
  - correct frequency dependence down to very low frequencies
  - „correct“ deviation from inexact NRG result



conclusion

- tensor networks for more realistic non-1D problems: use in DMFT
  - perform very well in difficult real systems
  - in imaginary time:
    - on the verge of outperforming competing approaches
    - should be able to access rare earth materials
    - analytical continuation issues
  - in real time:
    - works, but spectral resolution insufficient
    - complex-time evolution may bring back real-time!