Application of Matrix Product States to Condensed Matter and Ultracold Gases

Salvatore R. Manmana

Institute for Theoretical Physics, Georg-August-University Göttingen

GEORG-AUGUST-UNIVERSITÄT
GÖTTINGEN

$[q,p]=i\hbar$

Entanglement in Strongly Correlated Systems
Benasque, February 21st – March 4th 2022

Some Reviews:

Matrix Product States (MPS – modern language):

The density-matrix renormalization group in the age of matrix product states

Ulrich Schollwöck

arXiv:1008.3477,
Annals of Phys. **326**, 96 (2011)

Time-evolution methods for matrix-product states

Sebastian Paeckel[a], Thomas Köhler[a,b], Andreas Swoboda[c], Salvatore R. Manmana[a], Ulrich Schollwöck[c,d], Claudius Hubig[e,d,*]

arXiv:1901.05824,
Annals of Phys. **411**, 167998 (2019)

Density Matrix Renormalization Group (DMRG – ‚old style')

The density-matrix renormalization group*

U. Schollwöck

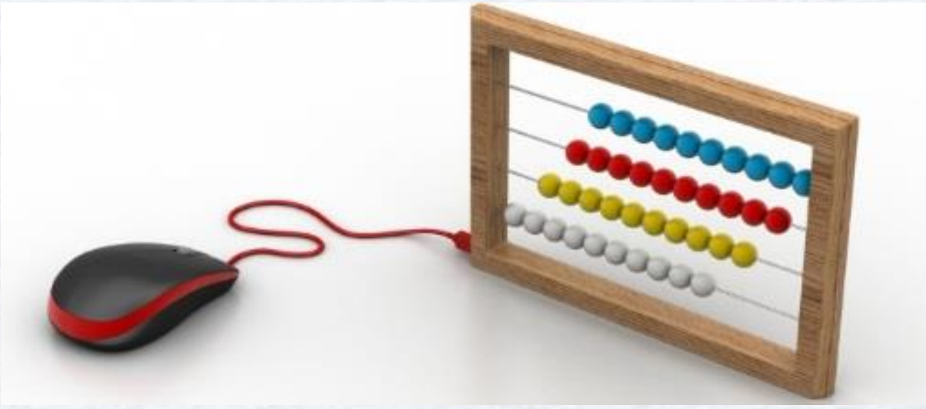
arXiv:cond-mat/0409292,
Rev. Mod. Phys. **77**, 259 (2005)

Diagonalization- and Numerical Renormalization-Group-Based Methods for Interacting Quantum Systems

Reinhard M. Noack* and Salvatore R. Manmana†,*

arXiv:cond-mat/0510321,
AIP Conf. Proc. **789**, 93 (2005)

Part I: General Overview



Quantum Many-Body Systems: Correlations

Correlated states:

"mean-field" picture of independent particles breaks down

$$\langle S_1^z S_2^z \rangle \neq \langle S_1^z \rangle \langle S_2^z \rangle + \langle (S_1^z - \langle S_1^z \rangle)(S_2^z - \langle S_2^z \rangle) \rangle$$

➠ Expectation values of observables for particles 1 and 2 *correlate with each other*

a) because of entanglement

b) because of mutual interactions.

Small numerical values: need *accurate* methods

Unconventional States: Topological Phases

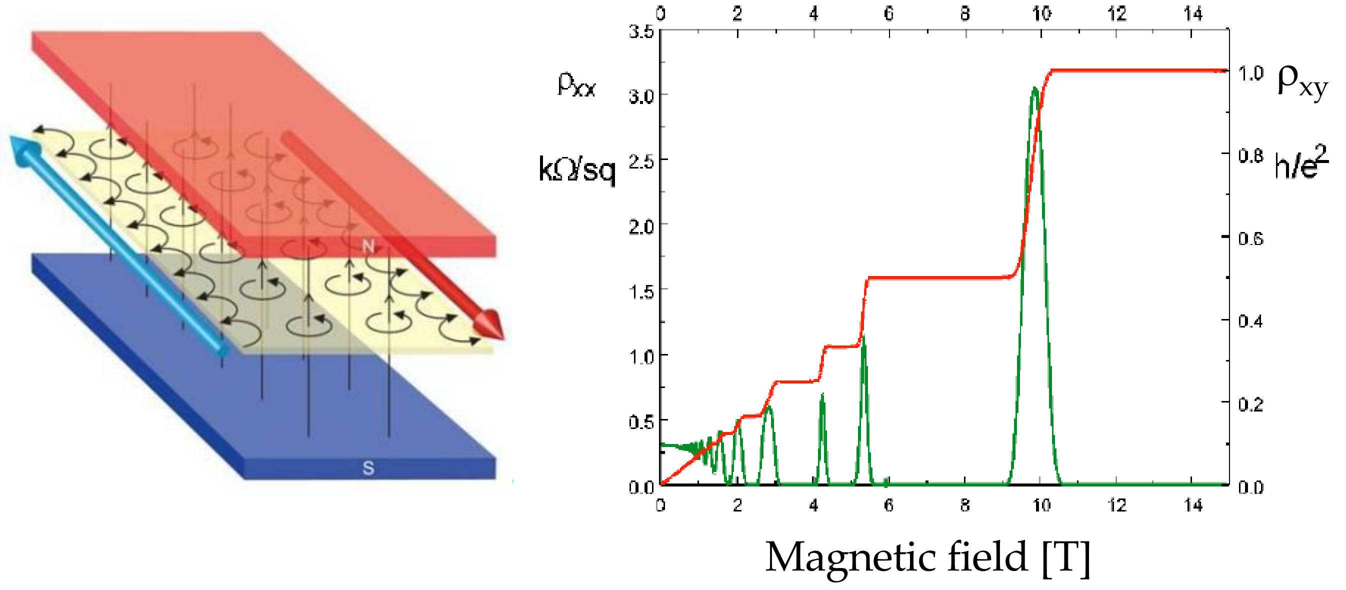
"Topological order": beyond Landau paradigm

Nobel Prize 2016

No local order parameter, instead:

- *topological invariants* (integer numbers)
  → protection against local noise: quantum computing
- metallic surface states
  → dissipationless transport

Examples: integer and fractional quantum Hall effect



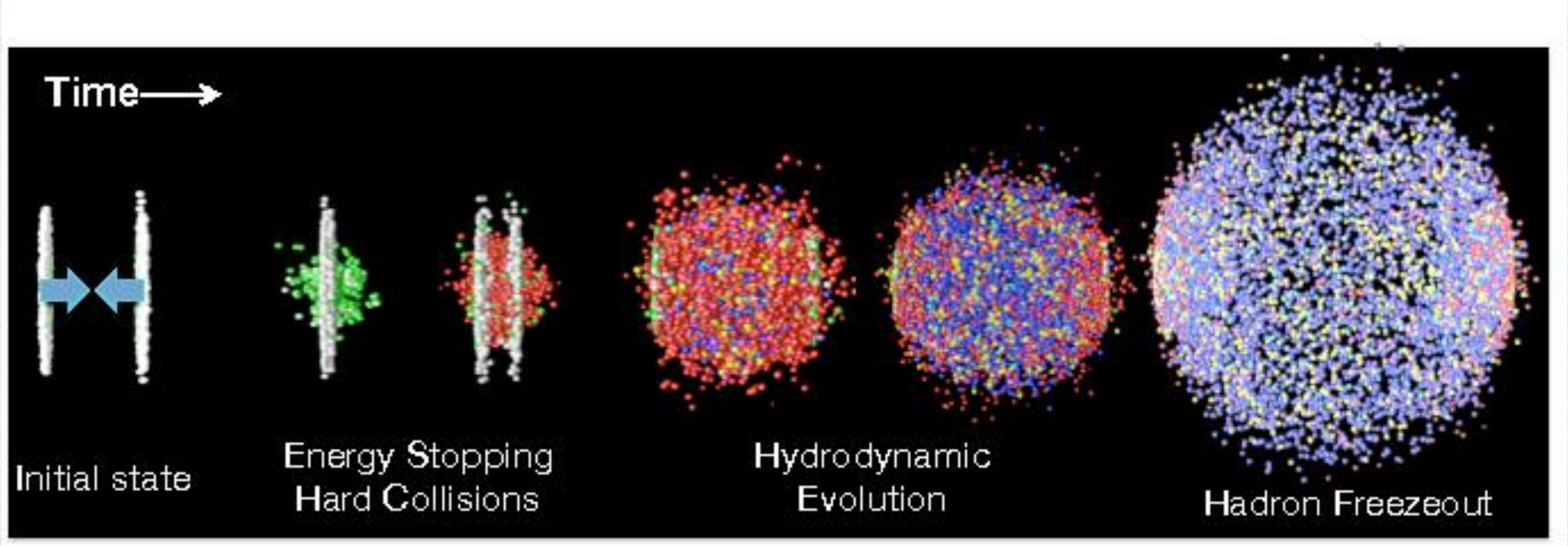
Phase transitions:
jumps in transverse conductivity

How to investigate this numerically? Which quantities to compute?

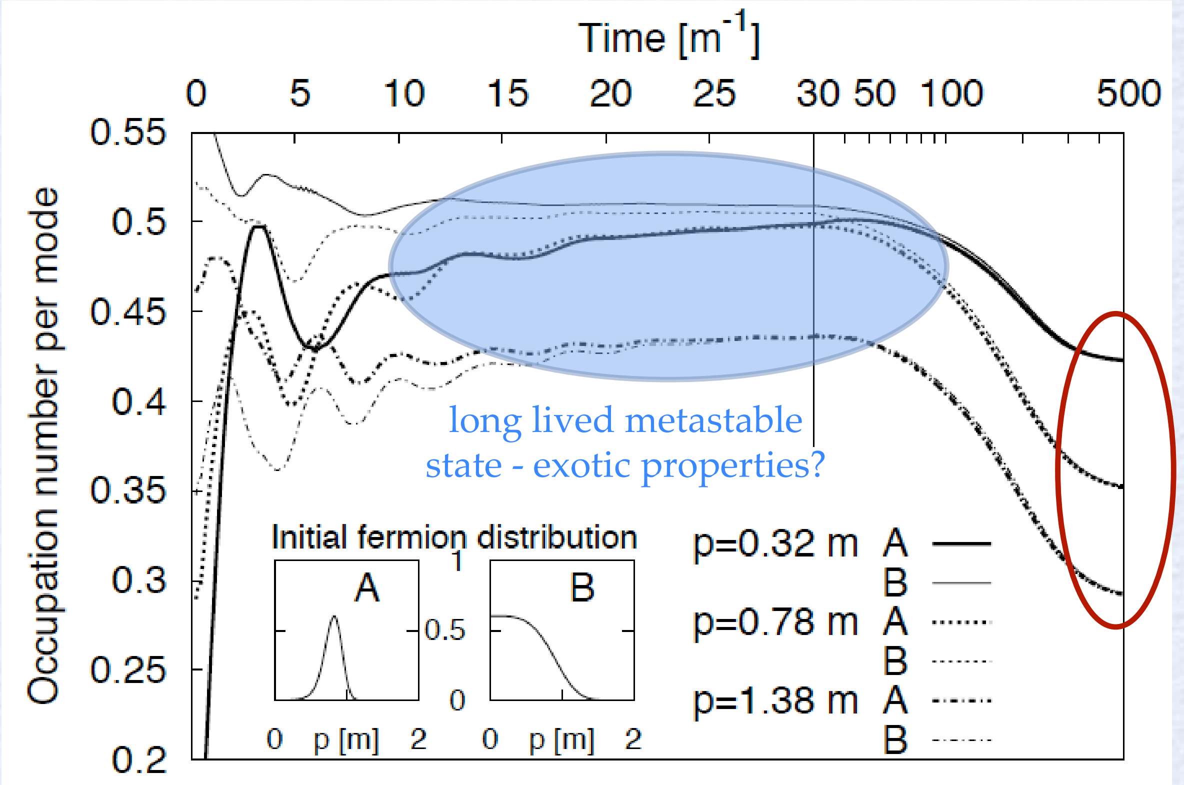
⇒ local observables, topological invariants, energy gaps, *entanglement* properties, „Schmidt spectrum",…

Unconventional states: Out-of-Equilibrium Dynamics

Example (high-energy physics):
heavy ion collisions



[from inspirehep.net]



thermal
final state

[Berges *et al.*, PRL 2004]

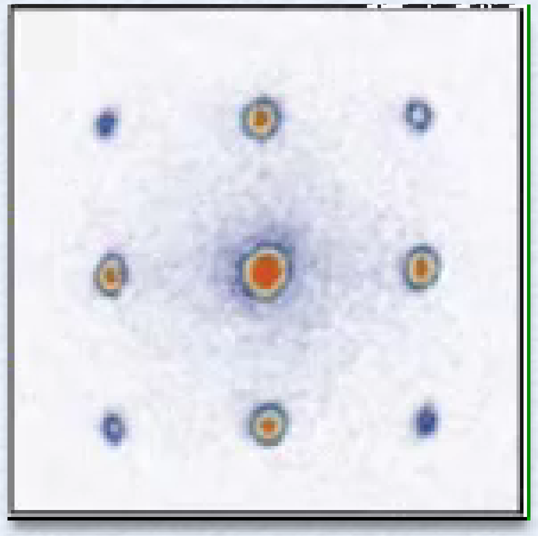
Fundamental questions:

- How does the system ‘relax’ towards a ‘stationary state’?
- Temperature in the system?
- „Prethermalization“

Quantum Simulators:
Controlled Quench Dynamics

Out-of-Equilibrium

"Quantum Quenches"
➟ Sudden change of parameters
$U_0 \rightarrow U$

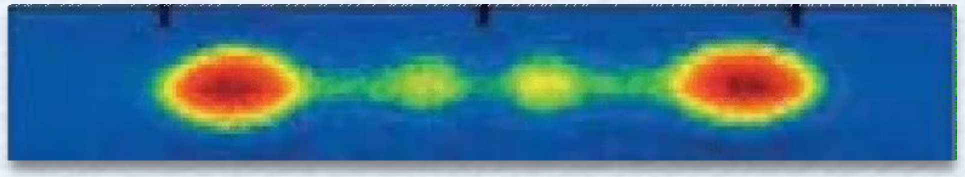


Collapse and Revival
of a Bose-Einstein-Condensate

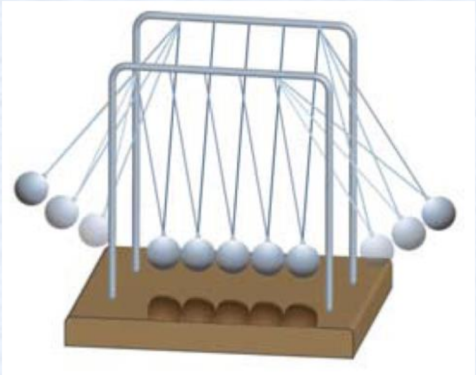
M. Greiner et al., Nature (2002)

Prepared states, Expansions

➟ "Release" atoms, remove a trapping potential



'Quantum Newton Cradle'



T. Kinoshita et al., Nature (2006)

- ➟ Relaxation behavior
- ➟ Time scales
- ➟ Non-Equilibrium states

How to investigate this numerically? Which quantities to compute?

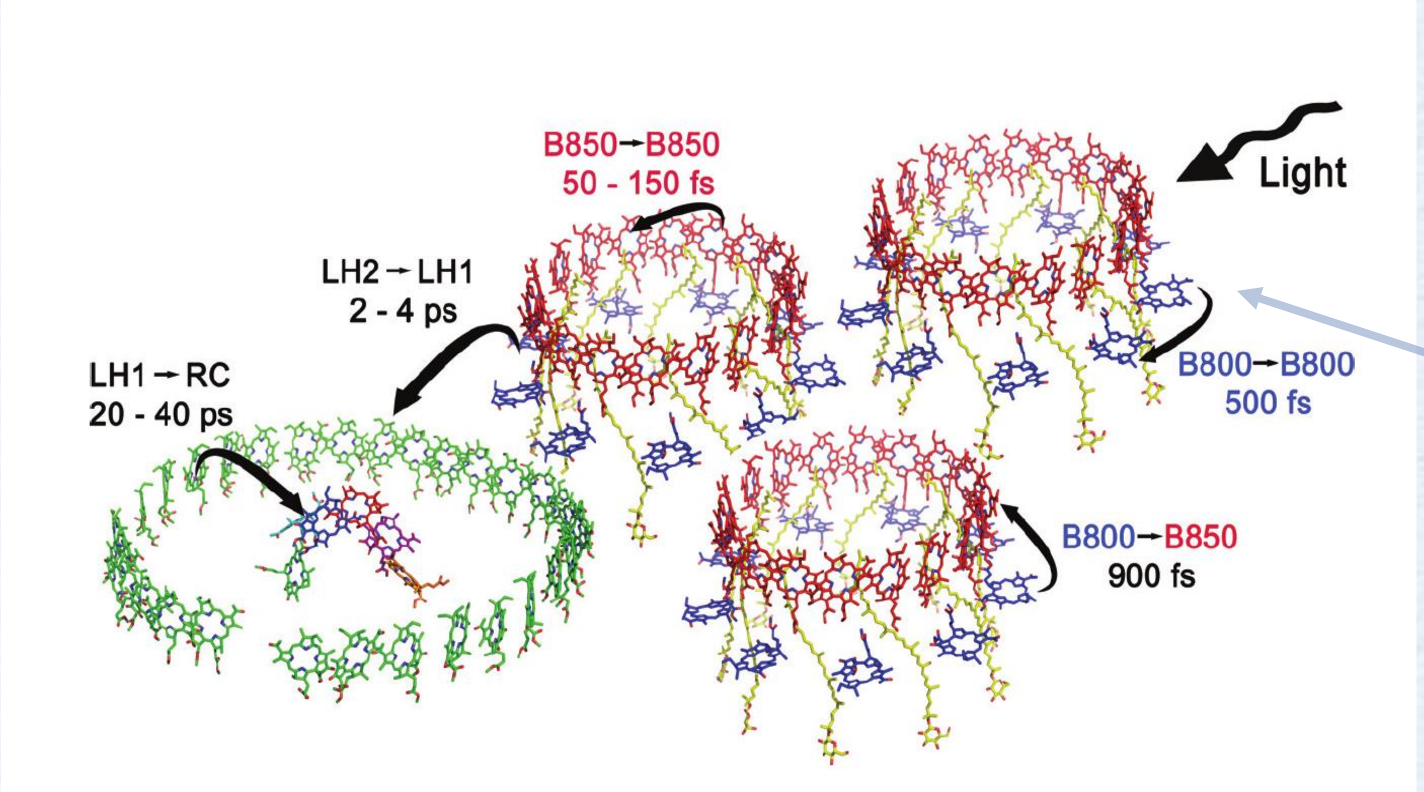
⇨ accurate methods for time evolution with time-independent Hamiltonians

Many-Body Systems Out-Of-Equilibrium: Phonons

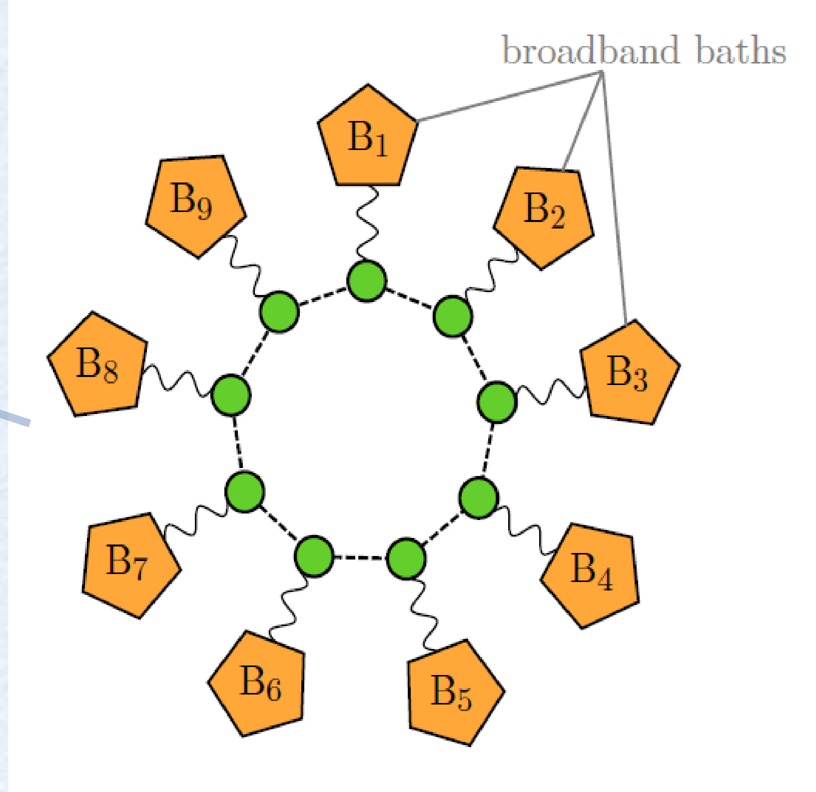
Example: light-harvesting systems

[R.K. Kessing, Master thesis (U. Göttingen, 2020); R. K. Kessing *et al.*, arXiv:2111.06137]

Energy transfer in ‚antenna systems‘



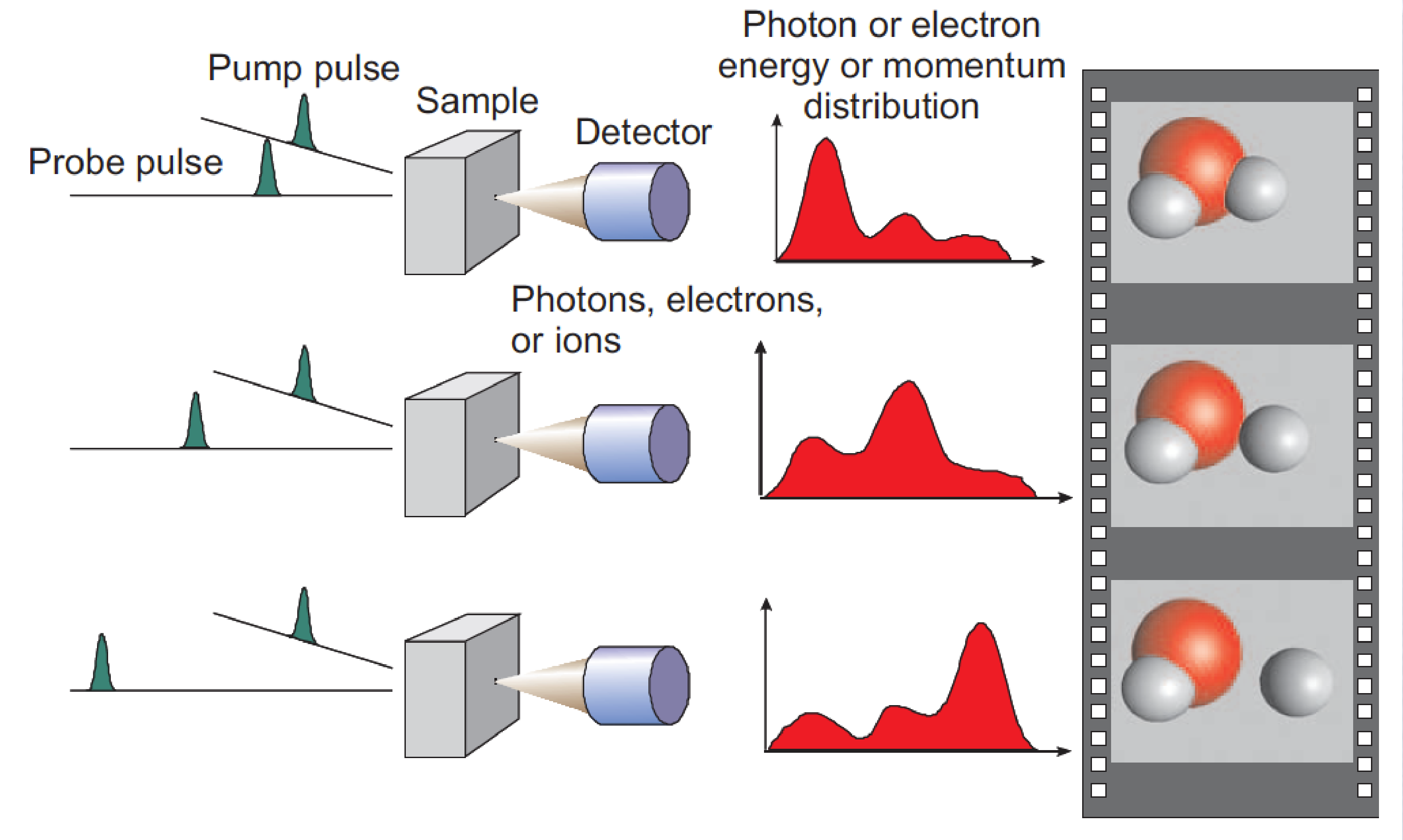
Simplified model:
ring geometry coupled to phonons



How to investigate this numerically? Which quantities to compute?

⇨ efficient approaches to treat phonons?

Many-Body Systems Out-Of-Equilibrium: Highly Excited Materials

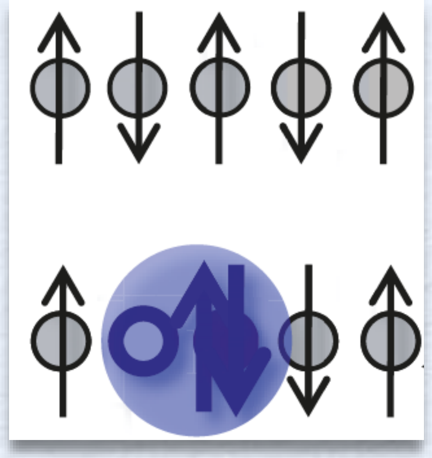


F. Krausz & M. Ivanov, RMP (2009)

How to investigate this numerically? Which quantities to compute?

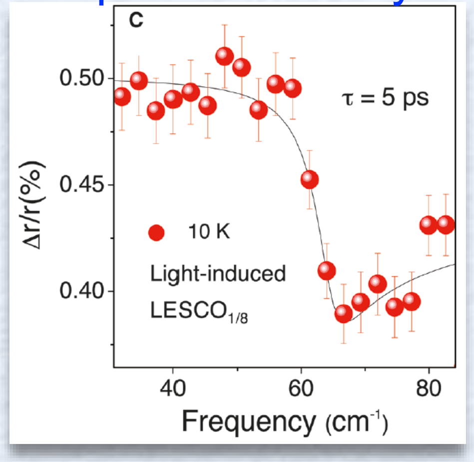
accurate methods for time evolution with *time-dependent* Hamiltonians, formation of order or quasiparticles?

Photo-excitation of Mott insulators



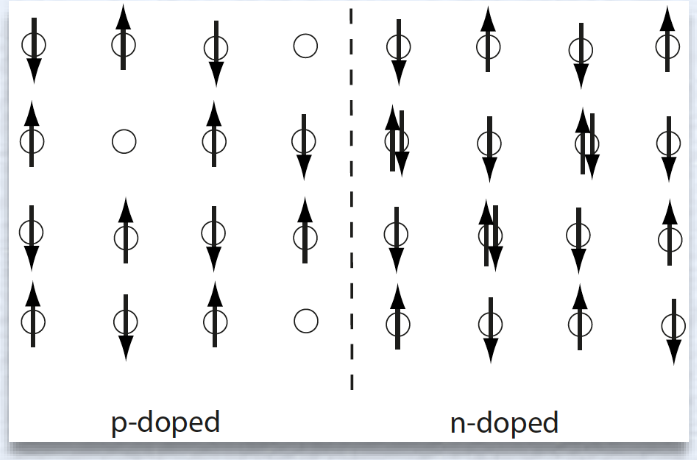
S. Wall et al., Nature Physics (2010)

“Light-induced superconductivity”



D. Fausti et al., Science (2011)

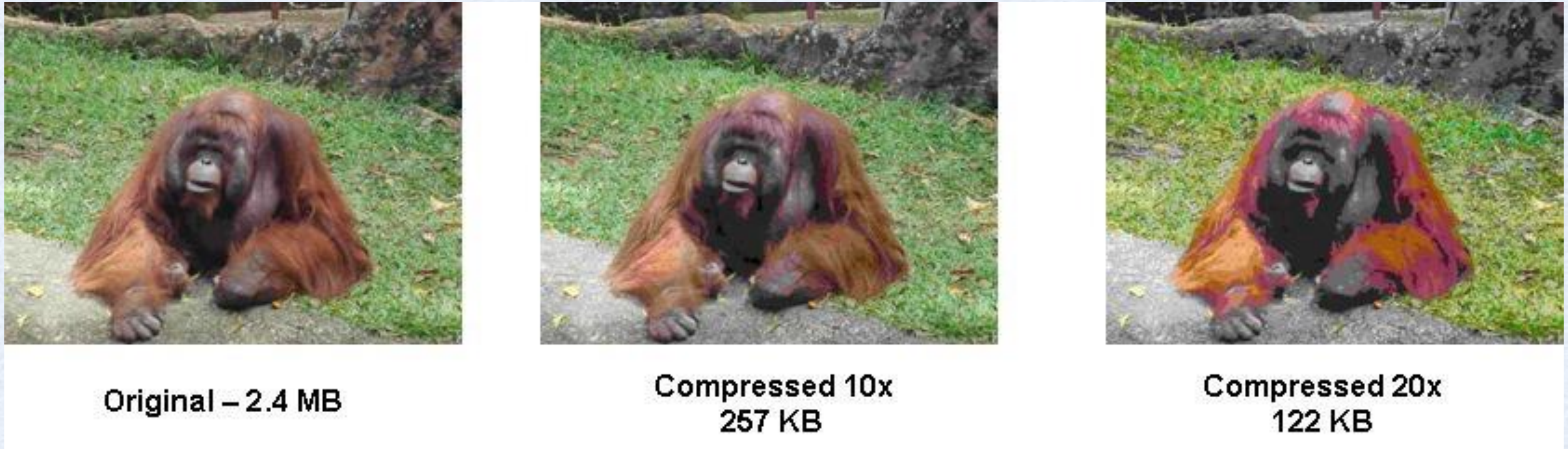
Photovoltaic effects



E. Manousakis PRB (2010)

DMRG, MPS and related methods:
Basic Idea

Basic idea: data compression (“quantum version”)



→ Graphics (acoustics, signal transmission, etc.)

Key aspect:
Ignore modes that cannot be resolved (by the ear, the screen, ...) – excellent quality with much smaller amount of data.

➠ Control parameter here: entanglement.

Matrix Product State: *Basic Idea*

[U. Schollwöck, Annals of Physics (2011)]

Wave function of a generic many-body system (e.g. S=1/2 chain):

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_N} c_{\sigma_1,\ldots,\sigma_N} |\sigma_1 \ldots \sigma_N\rangle$$

➟ 2^N coefficients (complex numbers)

Rewrite (using singular value decomposition, SVD):

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_N} \mathbf{A}^{\sigma_1}\mathbf{A}^{\sigma_2}\ldots\mathbf{A}^{\sigma_{N-1}}\mathbf{A}^{\sigma_N} |\sigma_1 \ldots \sigma_N\rangle$$

➟ $2 \cdot N$ matrices

Matrix Product State: Basic Idea

[U. Schollwöck, Annals of Physics (2011)]

MPS representation: local representation

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_N} \mathbf{A}^{\sigma_1}\mathbf{A}^{\sigma_2}\cdots\mathbf{A}^{\sigma_{N-1}}\mathbf{A}^{\sigma_N}\,|\sigma_1\ldots\sigma_N\rangle$$

Typical question: what‘s the gain? Don‘t we still have 2^N basis coefficients?

Consider the following two aspects:

1. We can *exploit* this **local representation** for the computation of expectation values – we do not need to store the coefficients, but only the matrices!

2. We can *truncate* the matrix size in a controlled way – we need to store only relatively small matrices and still obtain a high accuracy!

Matrix Product State: Basic Idea

[U. Schollwöck, Annals of Physics (2011)]

MPS representation: local representation

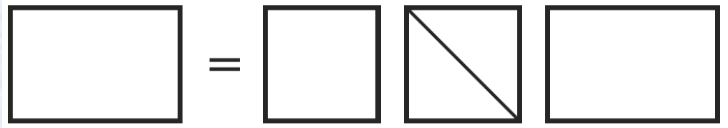
$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_N} \mathbf{A}^{\sigma_1}\mathbf{A}^{\sigma_2}\cdots\mathbf{A}^{\sigma_{N-1}}\mathbf{A}^{\sigma_N}\,|\sigma_1\ldots\sigma_N\rangle$$

Hence, we have two goals:

1. How do we obtain these matrices?
2. How do we compute all the interesting properties listed before?

How to rewrite a wave function to MPS form

1) Starting point: $|\psi\rangle = \sum_{\sigma_1,\dots,\sigma_N} c_{\sigma_1,\dots,\sigma_N} |\sigma_1 \dots \sigma_N\rangle$

2) Singular value decomposition (SVD): $\mathbf{M} = \mathbf{USV}^\dagger$ ➡ 

3) Rewrite coefficients:

$$c_{\sigma_1,\dots,\sigma_N} = \psi_{(\sigma_1),(\sigma_2,\dots,\sigma_N)} \overset{\text{SVD}}{=} \sum_{a_1}^{r_1} U_{\sigma_1,a_1} s_{a_1} \left(V^\dagger\right)_{a_1,(\sigma_2,\dots,\sigma_N)} \equiv \sum_{a_1}^{r_1} A^{\sigma_1}_{a_1} \psi_{(a_1\sigma_2),(\sigma_3,\dots,\sigma_N)}$$

4) Repeat until you reach the end:

$$c_{\sigma_1,\dots,\sigma_N} = \sum_{a_1}^{r_1} \sum_{a_2}^{r_2} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1,a_2} \psi_{(a_2\sigma_3),(\sigma_4,\dots,\sigma_N)}$$

$$\Rightarrow \quad |\psi\rangle = \sum_{\sigma_1,\dots,\sigma_N} \sum_{a_1,\dots,a_{N-1}} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1,a_2} \cdots A^{\sigma_{N-1}}_{a_{N-2},a_{N-1}} A^{\sigma_N}_{a_{N-1}} |\sigma_1 \dots \sigma_N\rangle$$

$$= \sum_{\sigma_1,\dots,\sigma_N} \mathbf{A}^{\sigma_1} \mathbf{A}^{\sigma_2} \cdots \mathbf{A}^{\sigma_{N-1}} \mathbf{A}^{\sigma_N} |\sigma_1 \dots \sigma_N\rangle \ ,$$

What about observables? Matrix Product Operators (MPO)

Similar to MPS ansatz: write operators as product of matrices

MPS:

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_N} \mathbf{A}^{\sigma_1}\mathbf{A}^{\sigma_2}\cdots\mathbf{A}^{\sigma_{N-1}}\mathbf{A}^{\sigma_N}\,|\sigma_1\ldots\sigma_N\rangle$$

MPO:

$$\widehat{O} = \sum_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} W^{\sigma_1\sigma'_1}W^{\sigma_2\sigma'_2}\ldots W^{\sigma_{L-1}\sigma'_{L-1}}W^{\sigma_L\sigma'_L}|\boldsymbol{\sigma}\rangle\langle\boldsymbol{\sigma}'|$$

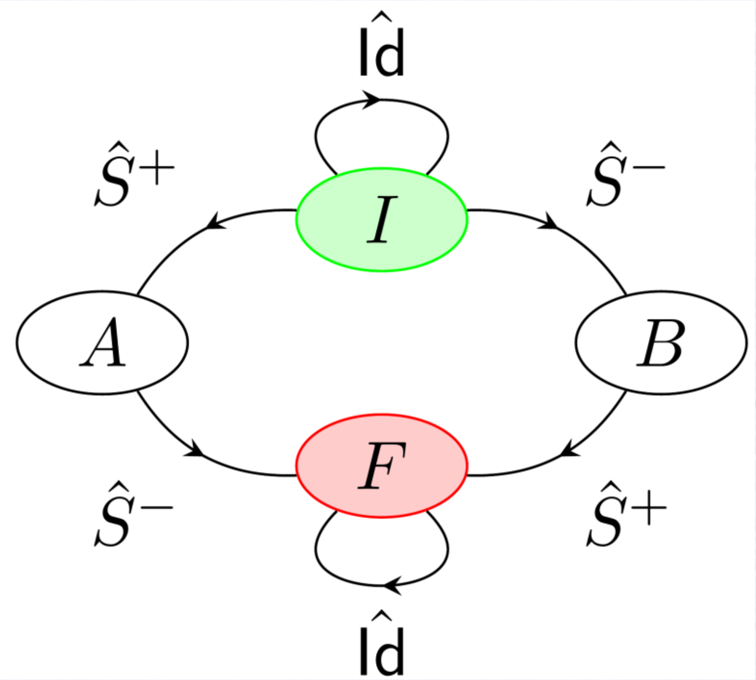
How to obtain these W matrices?

Useful representation of MPO-matrices: Finite states machines

[G.M. Crosswhite & D. Bacon, PRA (2008); G.M. Crosswhite et al. PRB (2008)]

$$\hat{H}_{XX} = \sum_i \hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+$$

$$\begin{array}{c c} & \begin{array}{cccc} I & A & B & F \end{array} \\ \begin{array}{c} I \\ A \\ B \\ F \end{array} & \begin{pmatrix} \hat{\mathrm{Id}} & \hat{S}^+ & \hat{S}^- & 0 \\ 0 & 0 & 0 & \hat{S}^- \\ 0 & 0 & 0 & \hat{S}^+ \\ 0 & 0 & 0 & \hat{\mathrm{Id}} \end{pmatrix} \end{array}$$



[Formulation with Abelian quantum numbers: S. Paeckel, T. Köhler & **S.R.M.**, SciPost Phys. 3, 035 (2017)

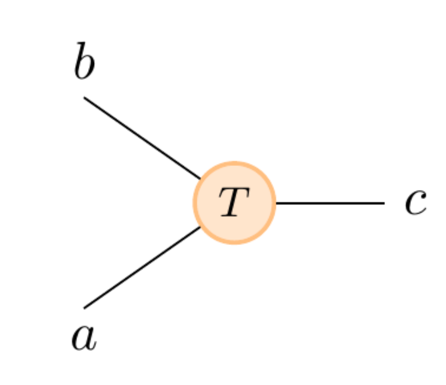
Freely available, flexible MPS code using FSM: https://www.symmps.eu]

Properties & Advantages:

- The FSM-graphs can be used as representation of the Hamiltonian/operator – unified input for all types of models possible
- Flexible control of time-dependence, 2D systems, observables,…
- Exact arithmethics by evaluation *after* construction of the operator

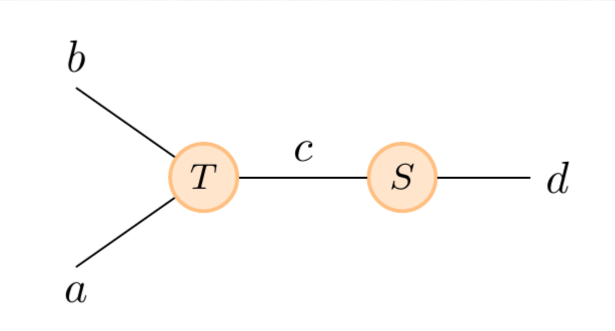
Good to know & very useful: Graphical Representation

„3-leg tensor“ (e.g., Matrix $\mathbf{A}^\sigma$):

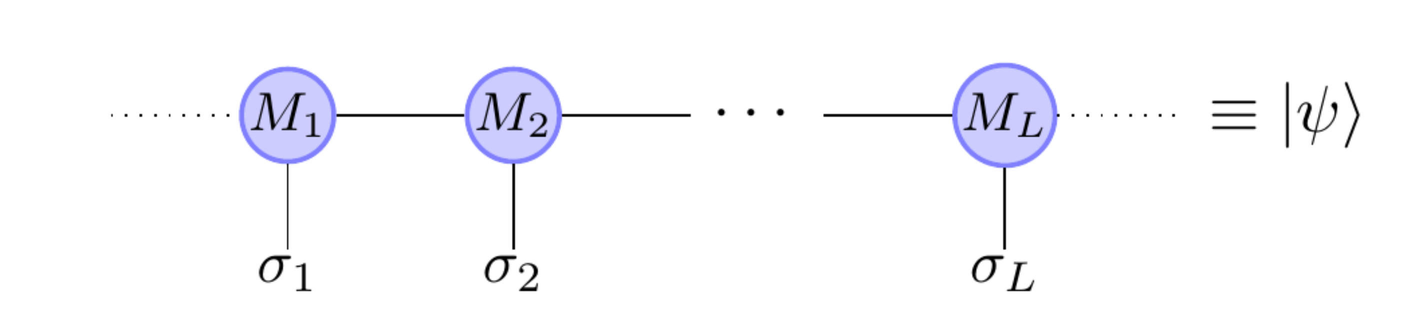


[This is also called *Penrose graphical notation of tensors*, R. Penrose (1971)]

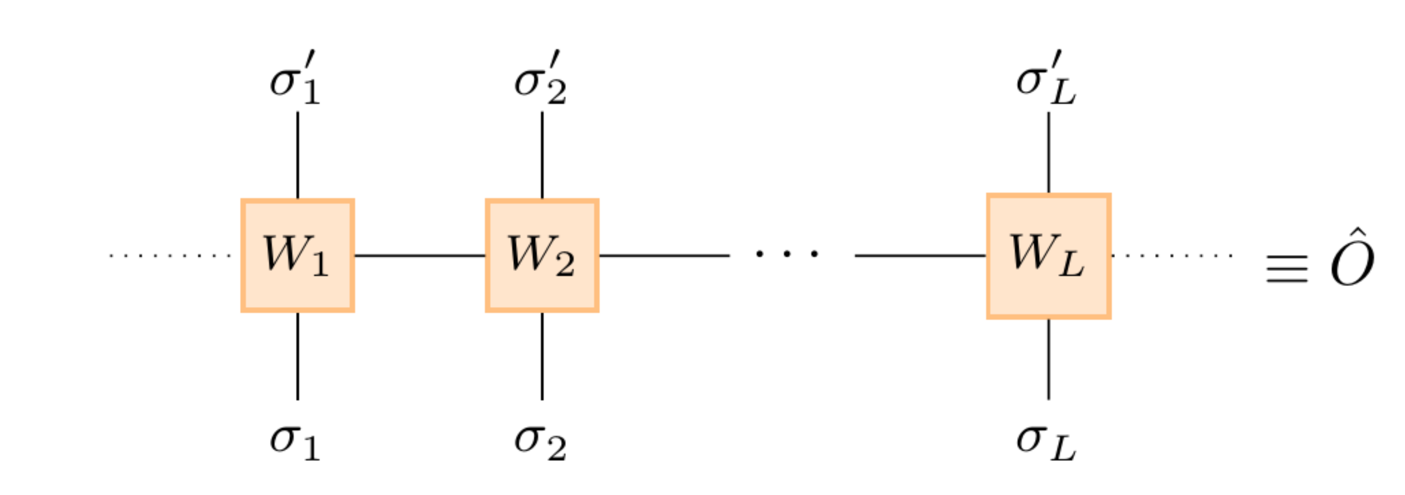
Contraction of two indices
(multiplication of two matrices)



Matrix Product State:



Matrix Product Operator:



Ground state search with MPS

[U. Schollwöck, Annals of Physics (2011)]

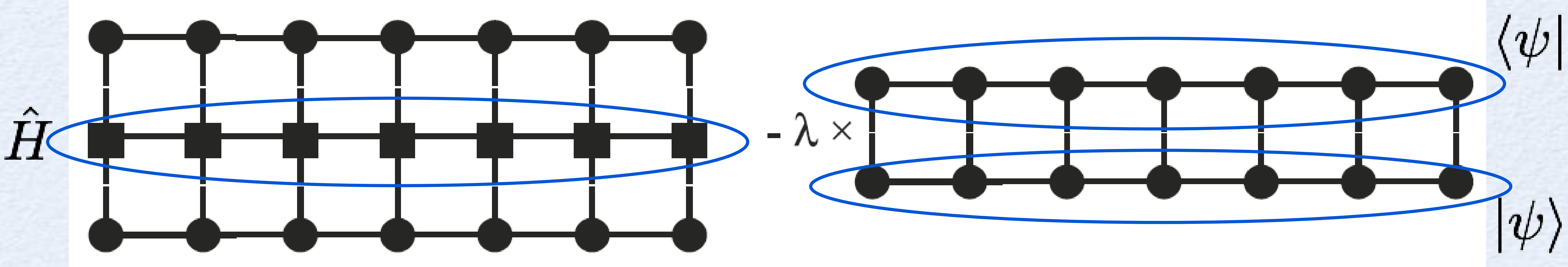
I) Imaginary time evolution until you reach the ground state

II) Iterative ground state search

Goal: Minimize

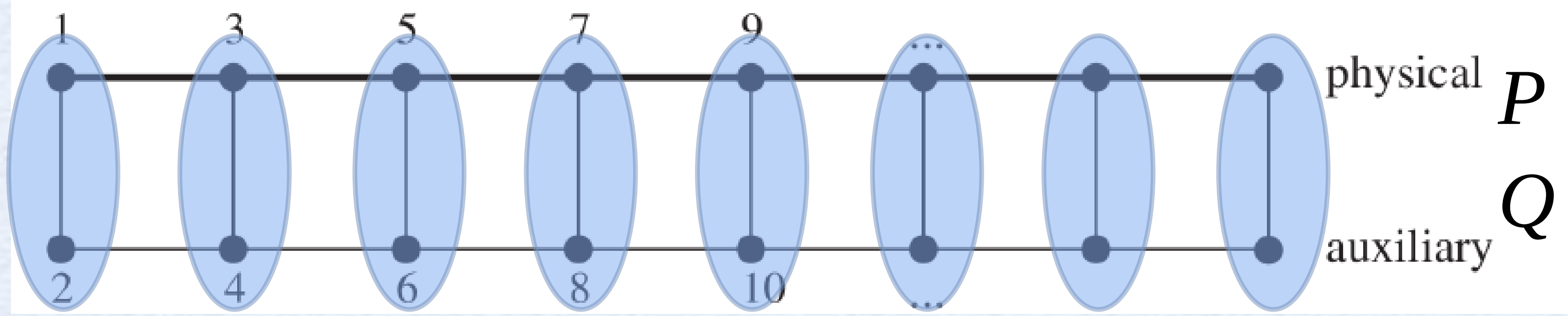
$$E = \frac{\langle\psi|\widehat{H}|\psi\rangle}{\langle\psi|\psi\rangle} \quad \Leftrightarrow \quad \langle\psi|\widehat{H}|\psi\rangle - \lambda\langle\psi|\psi\rangle$$

expectation value — scalar product



Finite temperature methods: purification & matrix product states

- Compute thermal density matrix via a pure state in an extended system:



formal replacement
$H \to H \otimes \mathbb{1}_Q$

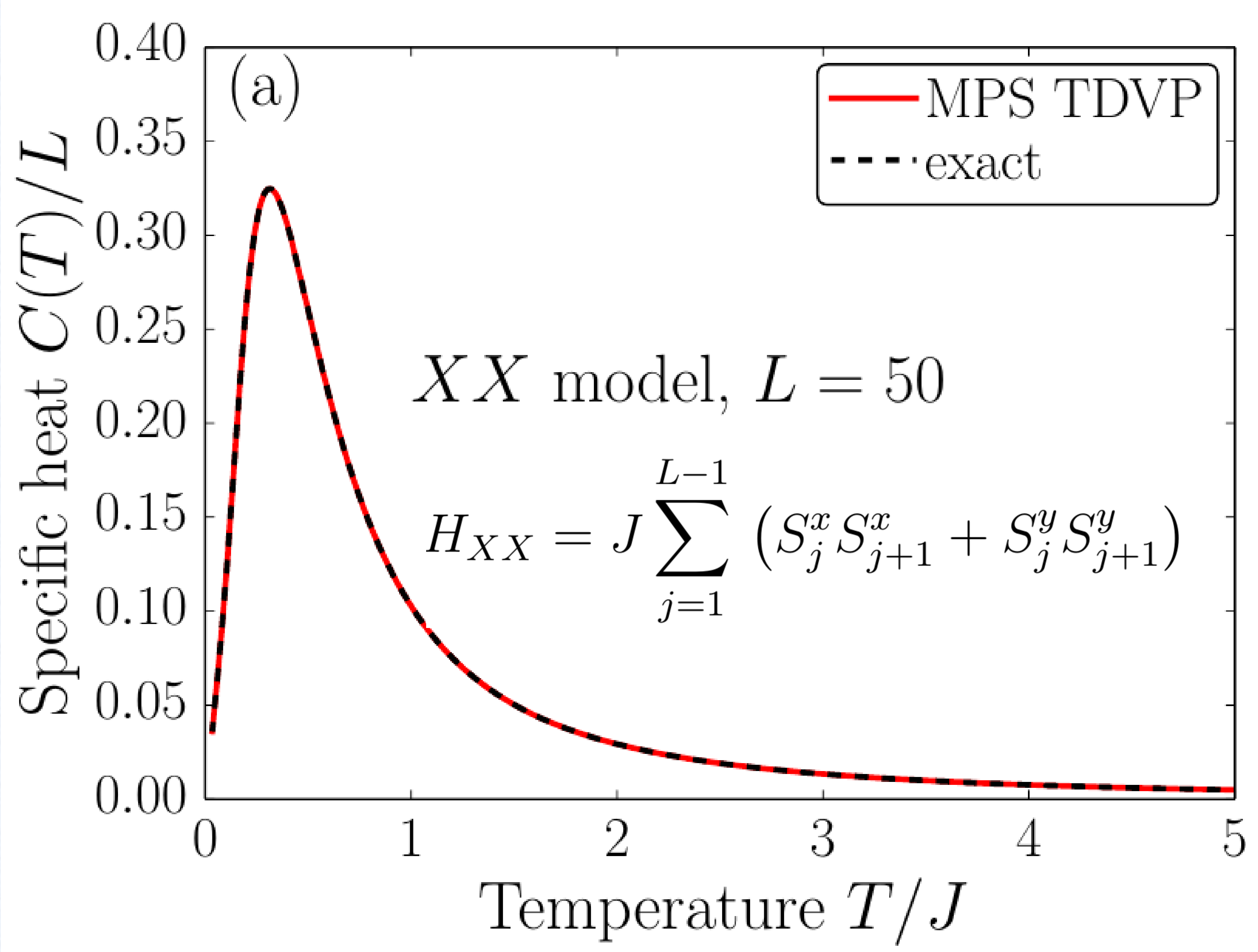
$$|\Psi_T\rangle \sim e^{-(H_P \otimes I_Q)/(2T)} \left[\otimes_{j=1}^{L} |\mathrm{rung}-\mathrm{singlet}\rangle_j \right]$$

$$\Rightarrow \varrho_T = \frac{1}{Z} e^{-H/T} = \frac{1}{Z} \mathrm{Tr}_Q |\Psi_T\rangle \langle \Psi_T|$$

Finite temperature methods: purification & matrix product states

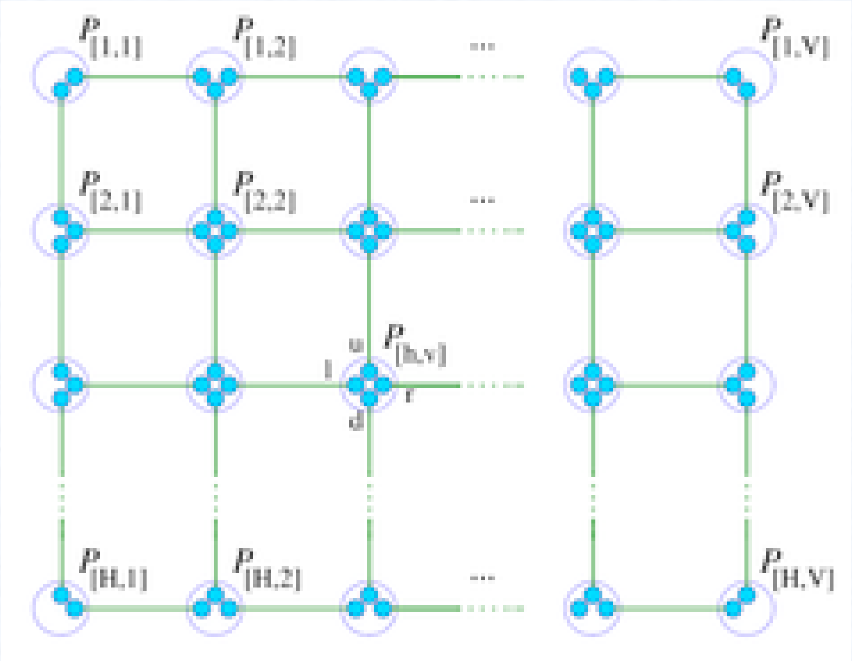
Example:

[A. Tiegel, PhD thesis (Göttingen, 2016)]



Outlook 2D:
PEPS, MERA & Tensor Networks

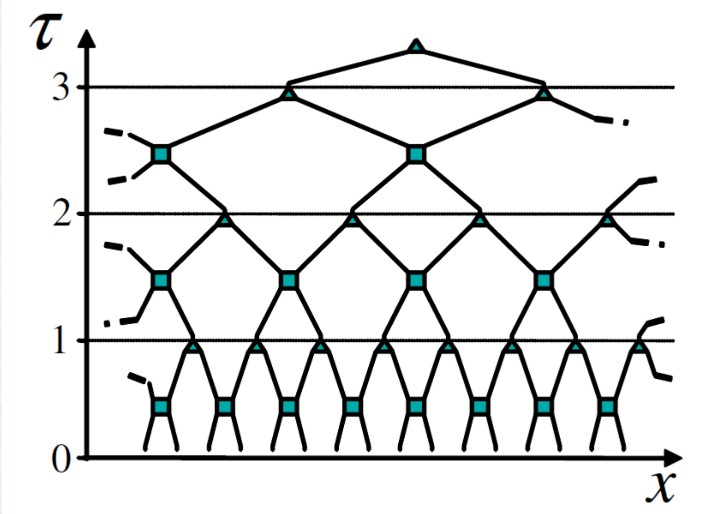
Projected Entangled Pair States (PEPS): F. Verstraete & I. Cirac, arXiv (2004)



$$|\psi\rangle = \sum_{k_1,\ldots,k_N=1}^{d} \mathcal{F}\left([A_1]^{k_1},\ldots,[A_N]^{k_N}\right)|k_1,\ldots,k_N\rangle$$

with $[A_i]^k_{l,r,u,d}$ *tensors (e.g., square lattice: rank-4)*

Multiscale Entanglement Renormalization Ansatz (MERA) & tensor networks: G. Vidal, PRL (2007)



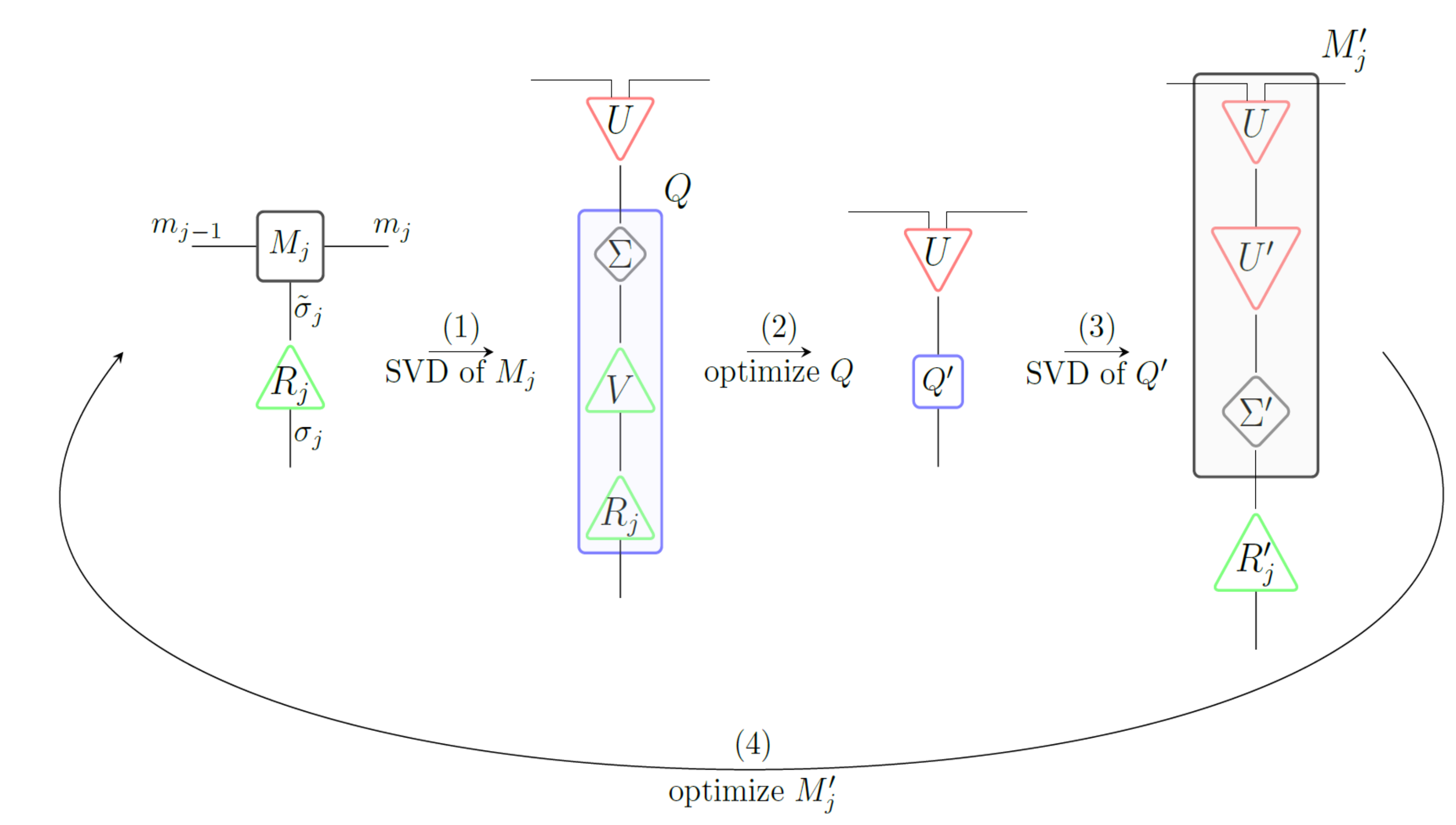
control of entanglement via unitary transforms:
'disentanglers' + block renormalization

Purification: quantum numbers for systems without conserved quantities

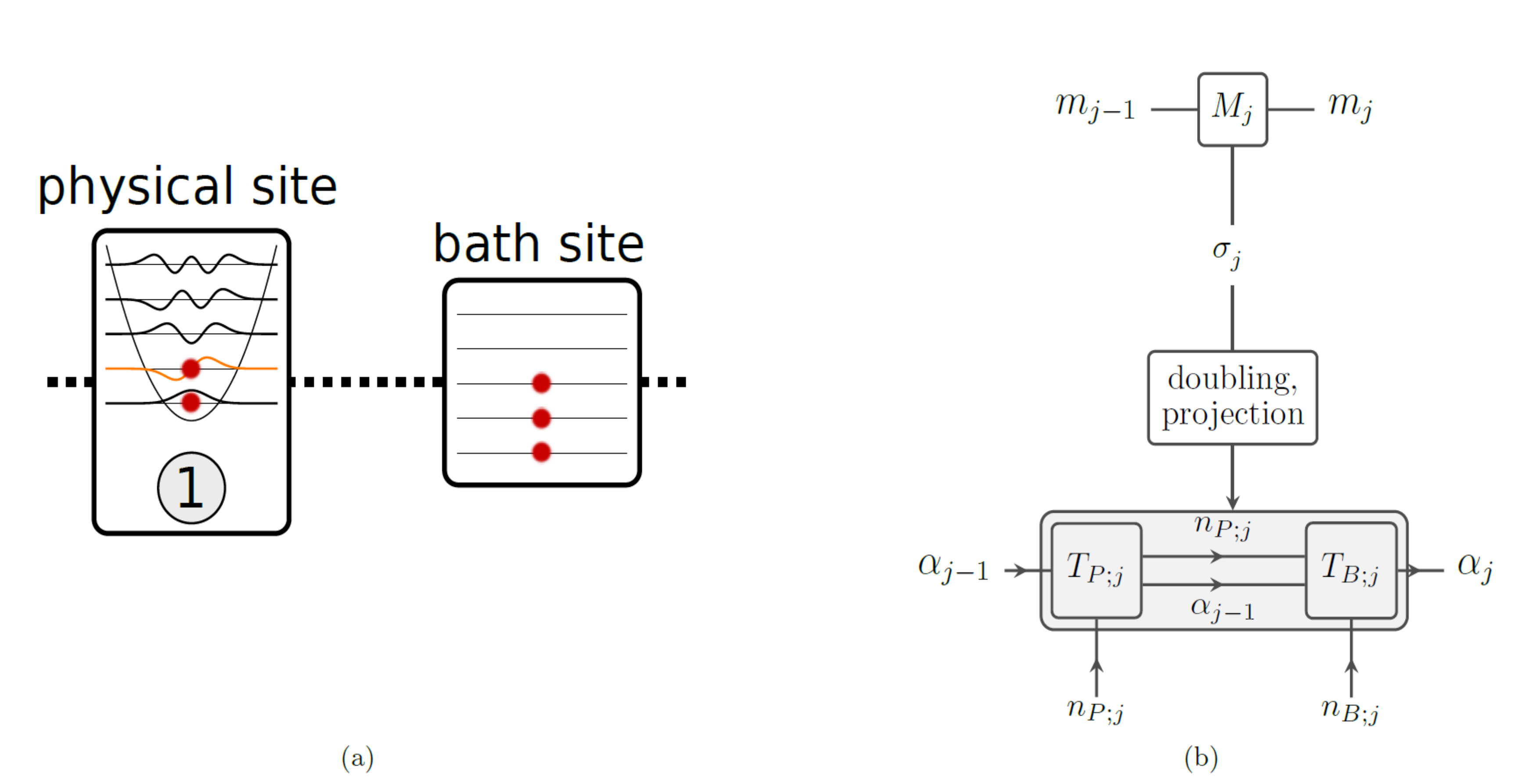
Comparison of methods: J. Stolpp et al., Comp. Phys. Comm. (2021)

Typical example: Holstein model $H = -t\sum_j \left(c_j^\dagger c_{j+1} + h.c.\right) + \omega_0 \sum_j b_j^\dagger b_j + \gamma \sum_j n_j^f \left(b_j^\dagger + b_j\right)$

Local basis optimization [e.g., C. Brockt et al. PRB (2015)]



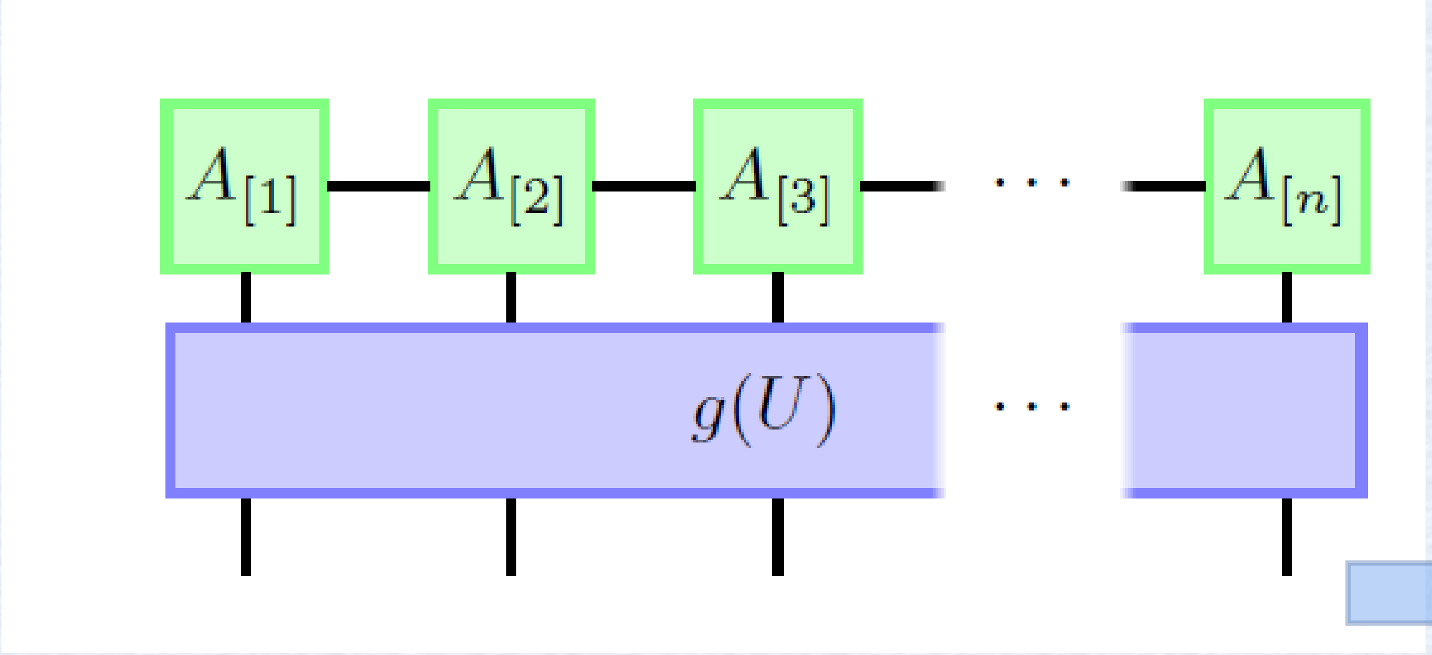
„pp-DMRG“ [T. Köhler, J. Stolpp & S. Paeckel SciPost (2021)]

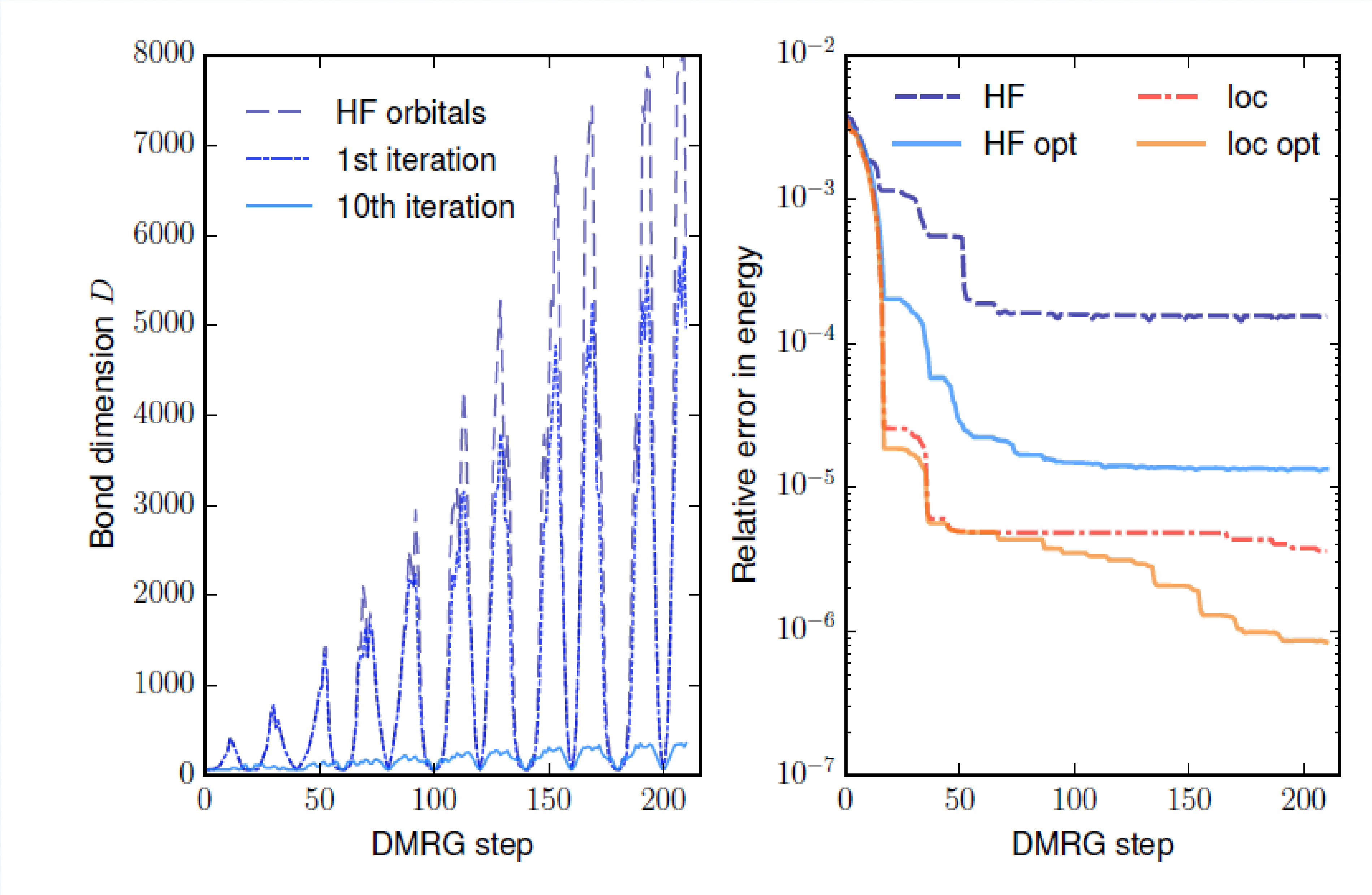


Significantly reduce the entanglement: ‚Mode Optimization‘

[C. Krumnow, L. Veis, Ö. Legeza & J. Eisert PRL (2016)]

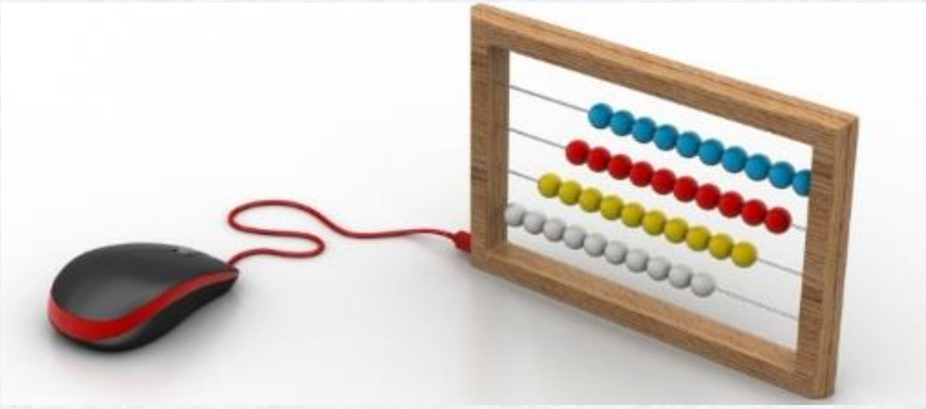
Idea: apply suitable unitary transform during the sweeps to go to a basis with smaller entanglement





Reduction of the bond dimension from 8000 to ~300 and improvement of the ground state energy!

Part II: Phase Diagrams and Topological Properties at $T=0$



Symmetry Protected Topological Phases

Possible characterization (X.-G. Wen):

➡ new kind of order at T=0

➡ SPT phases possess a symmetry and a finite energy gap.

➡ SPT states are short-range entangled states with a symmetry.

➡ defining properties:

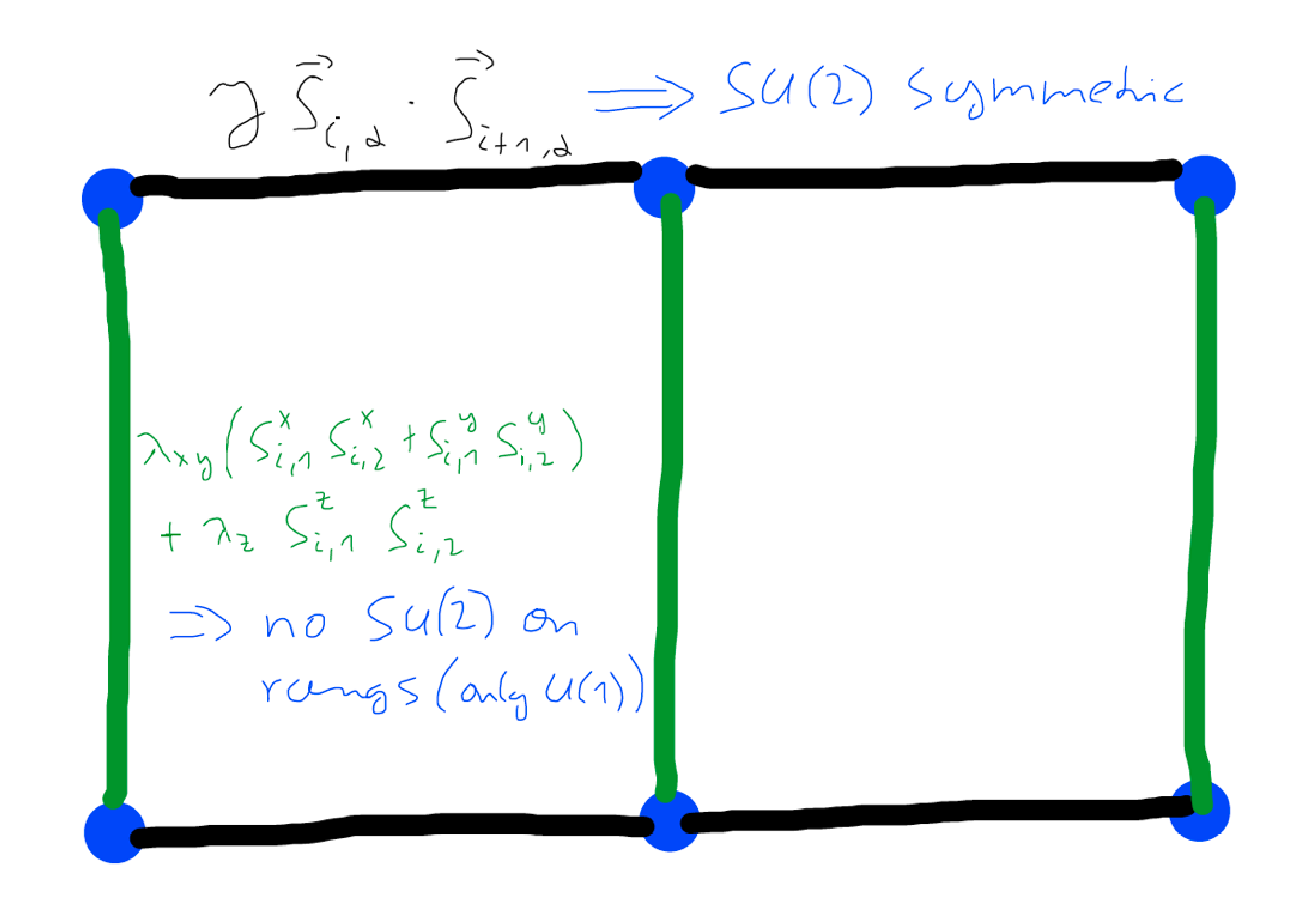
(a) distinct SPT states with a given symmetry cannot smoothly deform into each other without phase transition, if the deformation preserves the symmetry.

(b) however, they all can smoothly deform into the same trivial product state without phase transition, if we break the symmetry during deformation.

Note: “Real” Topological Phases ➡ “long-range entanglement” (Wen)

➡ What happens for long-ranged H?

Simple System with two SPT Phases



Analysis of "Wen's model"

Characterize topological phases via "entanglement spectrum":

F. Pollmann, A. Turner, E. Berg, and M. Oshikawa, PRB **81**, 064439 (2010)

A $\|\alpha\rangle_j$	B $\|\beta\rangle_j$

$$|\psi\rangle = \sum_{j=1}^{\dim\mathcal{H}} \sqrt{\lambda_j}\, |\alpha\rangle_j\, |\beta\rangle_j$$

λ_j: eigenvalues reduced density matrix, give entanglement spectrum

"Entanglement Splitting" test for 2-fold degeneracy:

$$ES = \sum_{j\,\mathrm{odd}} (\lambda_j - \lambda_{j+1})$$

test topological properties!

- staggered magnetization along the legs:

$$\langle m \rangle = \langle S^z_{L/2,\,1} \rangle - \langle S^z_{L/2+1,\,1} \rangle$$

- Spin gaps:

singlet gap: $\Delta^0_S = E_1(S^z_{\mathrm{total}} = 0) - E_0(S^z_{\mathrm{total}} = 0)$

triplet gap: $\Delta^1_S = E_0(S^z_{\mathrm{total}} = 1) - E_0(S^z_{\mathrm{total}} = 0)$

2nd triplet gap: $\Delta^{1,2}_S = E_0(S^z_{\mathrm{total}} = 2) - E_0(S^z_{\mathrm{total}} = 1)$

Analysis of "Wen's model"

[Z.-X. Liu, Z.-B. Yang, Y.-J. Han, W. Yi, and X.-G. Wen, PRB (2012)]

Symmetry of the ladder: $D_2 \times \sigma$(D_2 = {E,R_x,R_y,R_z}; σ: rung exchange)

➠ 8 distinct SPT phases: from projective representations, characterized via 'active operators'

	R_z	R_x	σ	Active operators	SPT phases
E_0	1	1	1		Rung-singlet[a], $t_x \times t_x, \ldots$
E_1	I	$i\sigma_z$	σ_y	(S_-^z, S_+^z, SS_-)	$t_x \times t_y$
E_2	σ_z	I	$i\sigma_y$	(S_-^x, S_+^x, SS_-)	$t_y \times t_z$
E_3	$i\sigma_z$	σ_x	I	(S_+^x, S_+^y, S_+^z)	$t_0, t_x \times t_y \times t_z$
E_4	σ_z	$i\sigma_z$	$i\sigma_x$	(S_+^y, S_-^y, SS_-)	$t_x \times t_z$
E_5	$i\sigma_z$	σ_x	$i\sigma_x$	(S_+^x, S_-^y, S_-^z)	t_x
E_6	$i\sigma_z$	$i\sigma_x$	σ_z	(S_-^x, S_-^y, S_+^z)	t_z
E_7	$i\sigma_z$	$i\sigma_x$	$i\sigma_y$	(S_-^x, S_+^y, S_-^z)	t_y

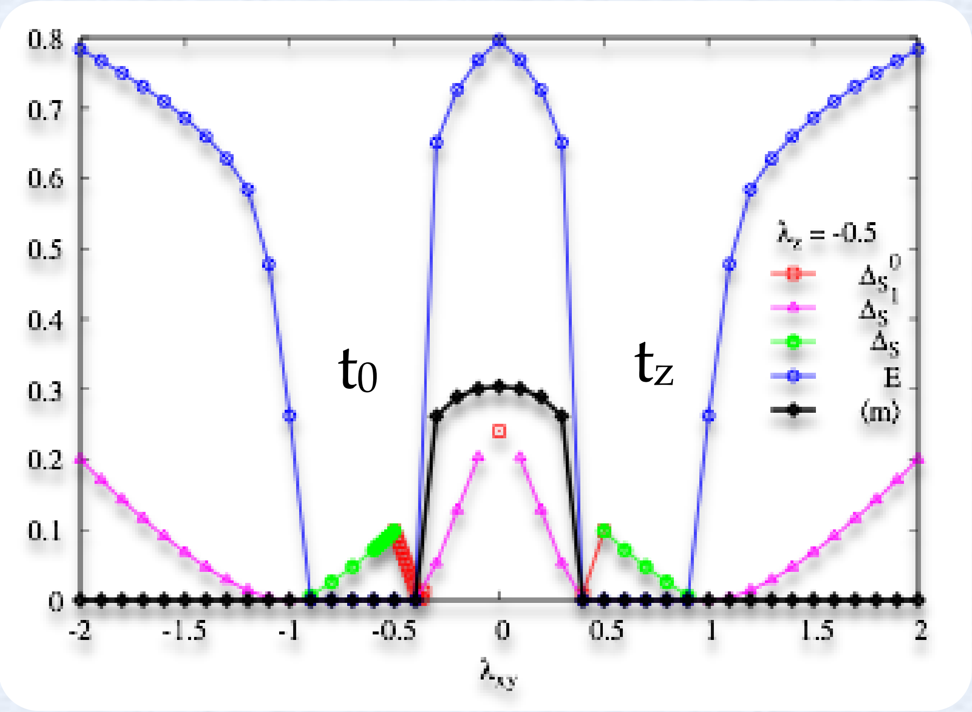
With $$O_\pm = O_1 \pm O_2$$

$$SS_- = \vec{S}_{i,1} \cdot \vec{S}_{i+1,1} - \vec{S}_{i,2} \cdot \vec{S}_{i+1,2}$$

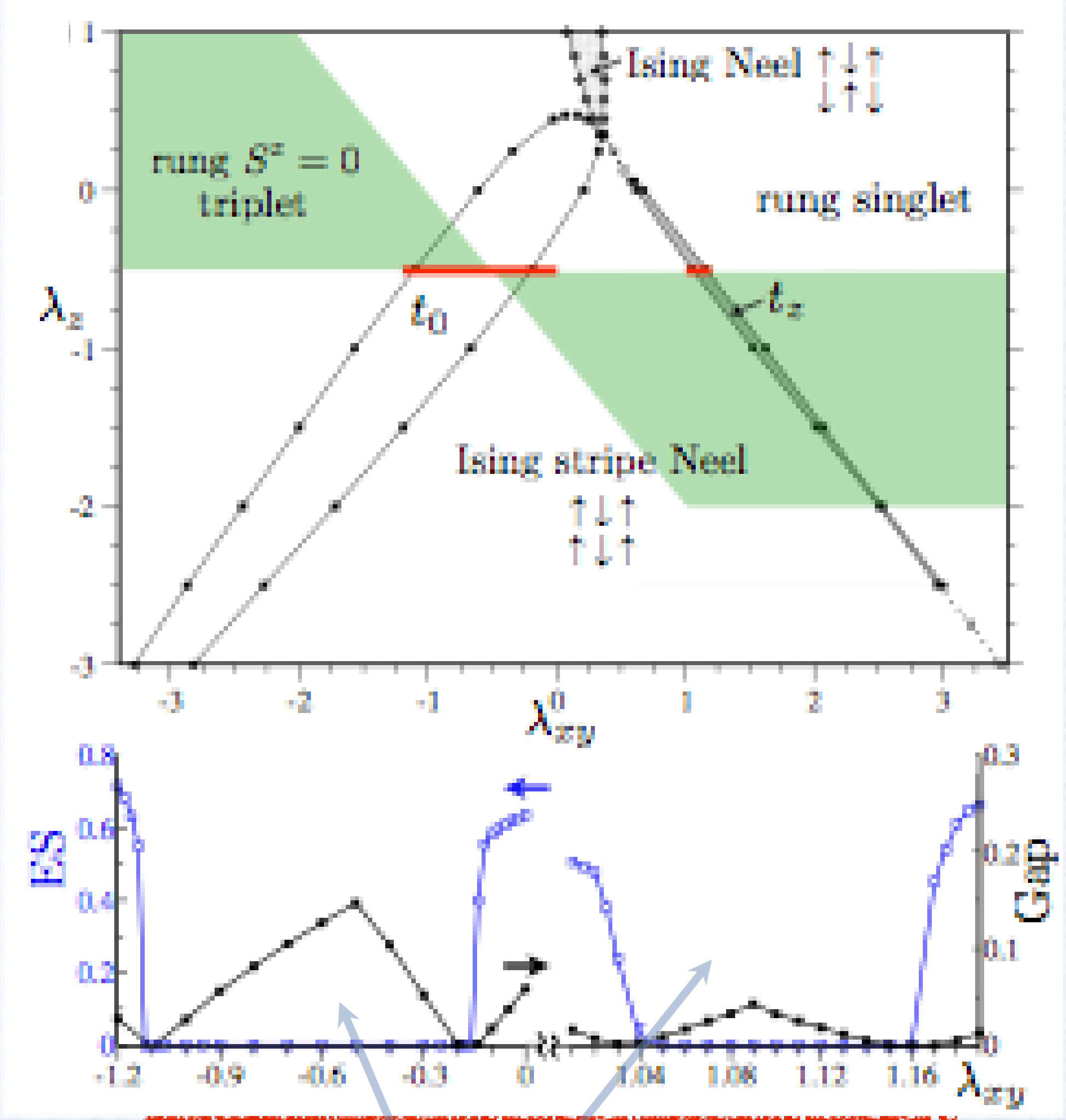
Phase Diagram without and with Long Range Interactions

S.R. Manmana et al., PRB (rapid comm.) **87,** 081106(R) (2013)

Nearest neighbor interactions:
(standard DMRG up to 400 rungs)



Long-range $1/r^3$ interactions:
(MPO, up to 400 rungs)



gapped + degenerate entanglement spectrum

Ground-state degeneracy:

t_0 phase:

$S_1^x+S_2^x$:
E_0 = -188.25372468551
E_1 = -188.24741526006

$S_1^x-S_2^x$:
E_0 = -188.24728807477
E_1 = -188.2472878754

t_z phase:

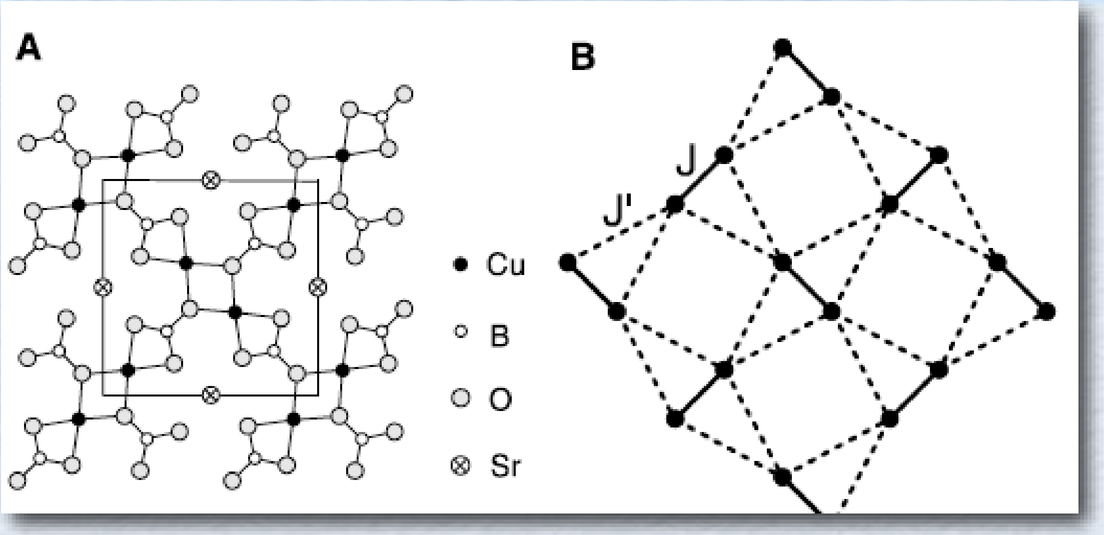
$S_1^x+S_2^x$:
E_0 = -188.24727291579
E_1 = -188.24727272182

$S_1^x-S_2^x$:
E_0 = -188.25372545779
E_1 = -188.24741603227

➠ SPT phases seem to persist in the presence of dipolar interactions

A highly frustrated quantum magnet: $SrCu_2(BO_3)_2$

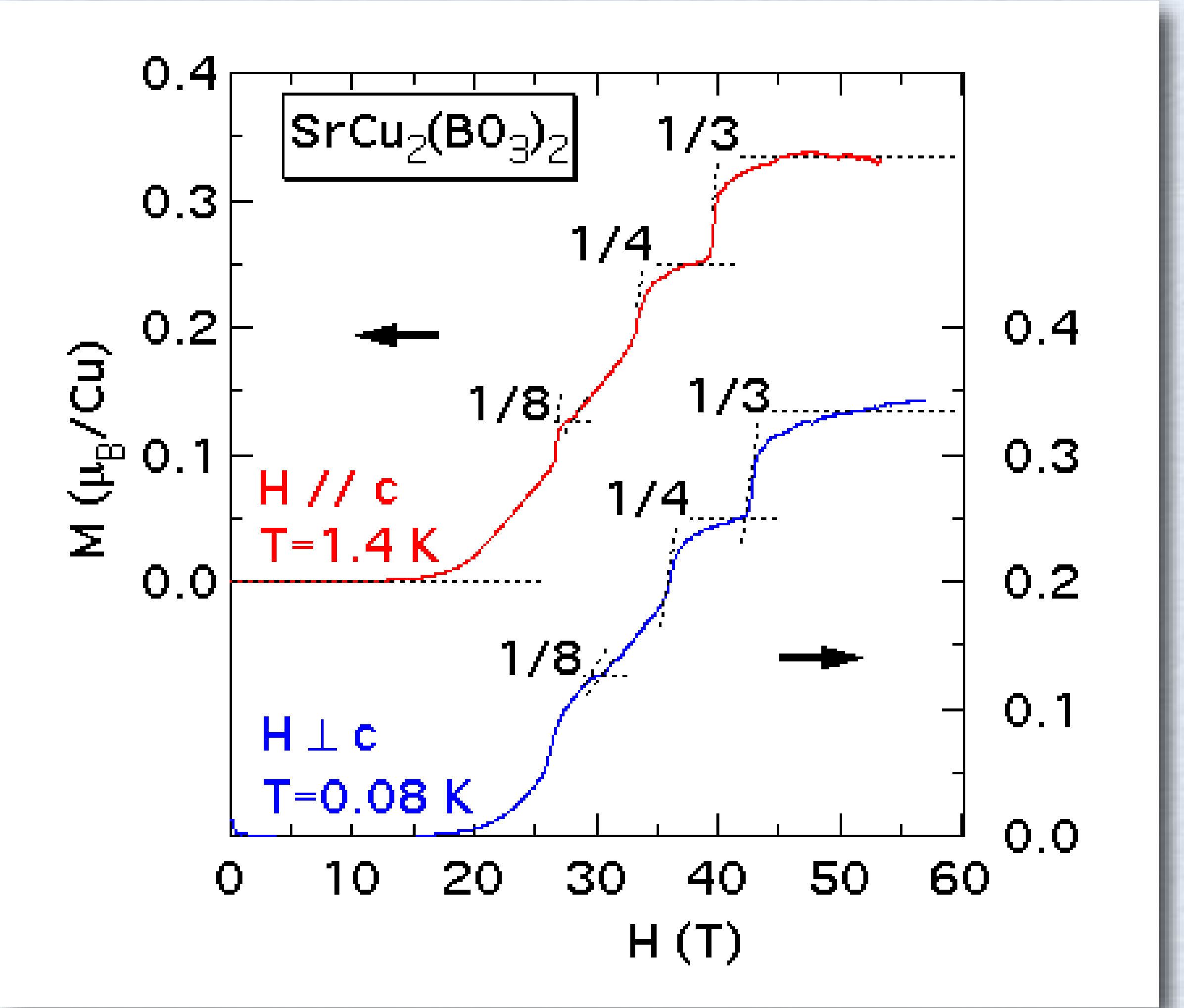
[H. Kageyama *et al.*, PRL **82**, 3168 (1999),
K. Kodama et al., Science **298**, 395 (2002)]



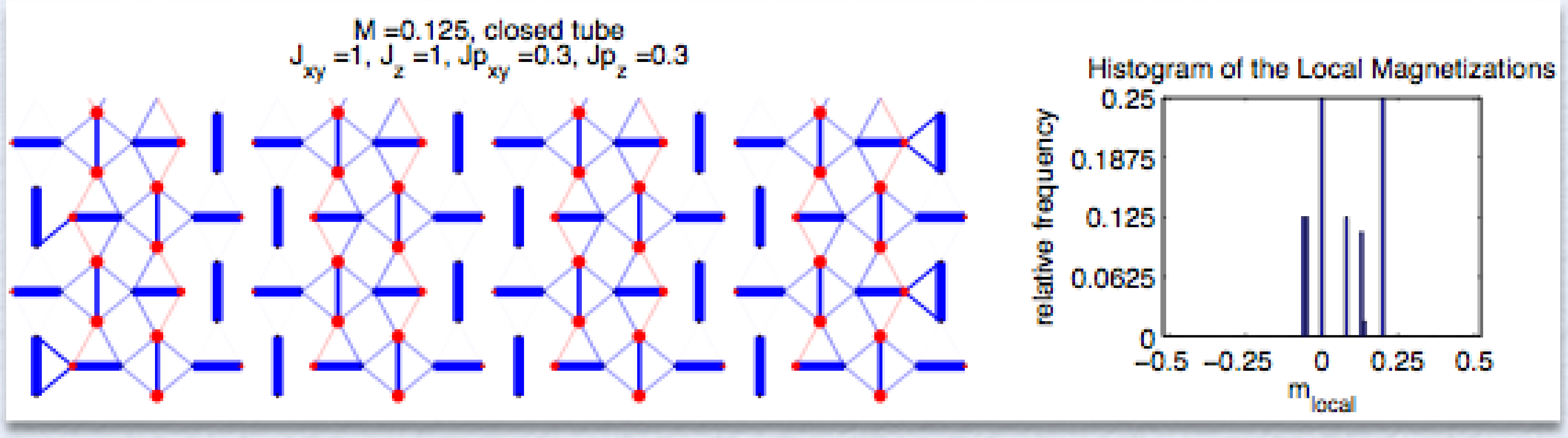
- Network of orthogonal dimers in a plane:

  2D Shastry-Sutherland lattice
- Series of fractional magnetization plateaux, e.g., at 1/8, 1/4, and 1/3 (+ further)
- Exotic states (e.g. spin-supersolid) in the vicinity or on the plateaux?
- Magnetization curve and plateaux at low fields are an ongoing challenge
- Theoretical treatment of the full 2D system very difficult

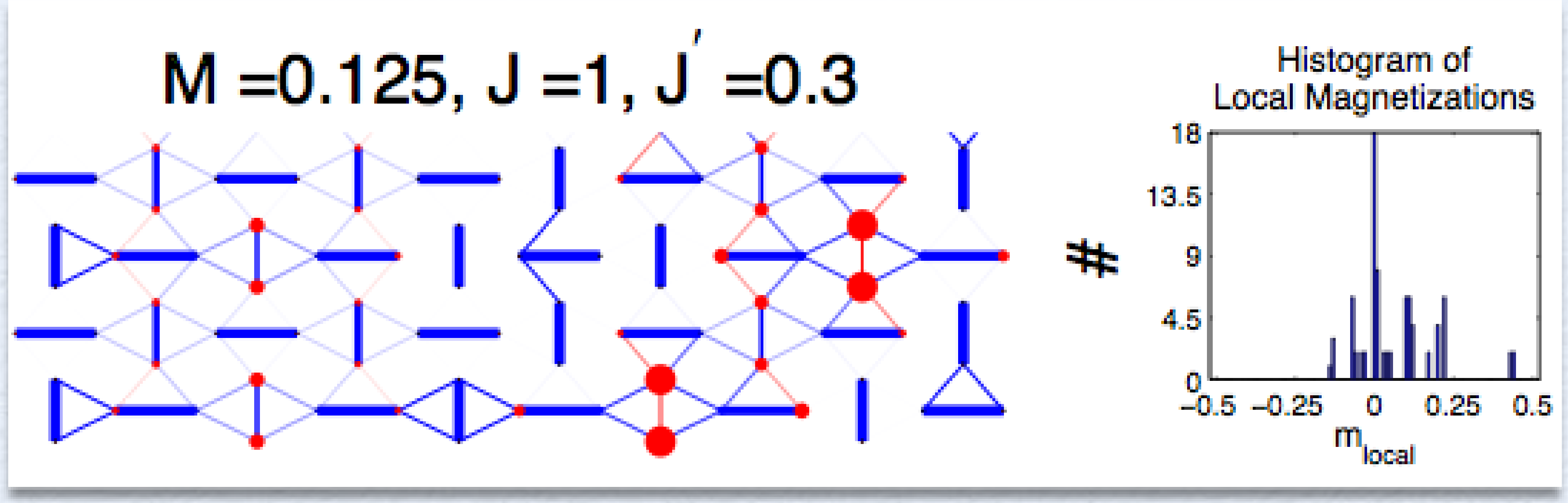
Here: Quasi-2D versions of this system



Quasi-2D Shastry-Sutherland lattice: DMRG on the 1/8 plateau



E/N = -0.319238530384945

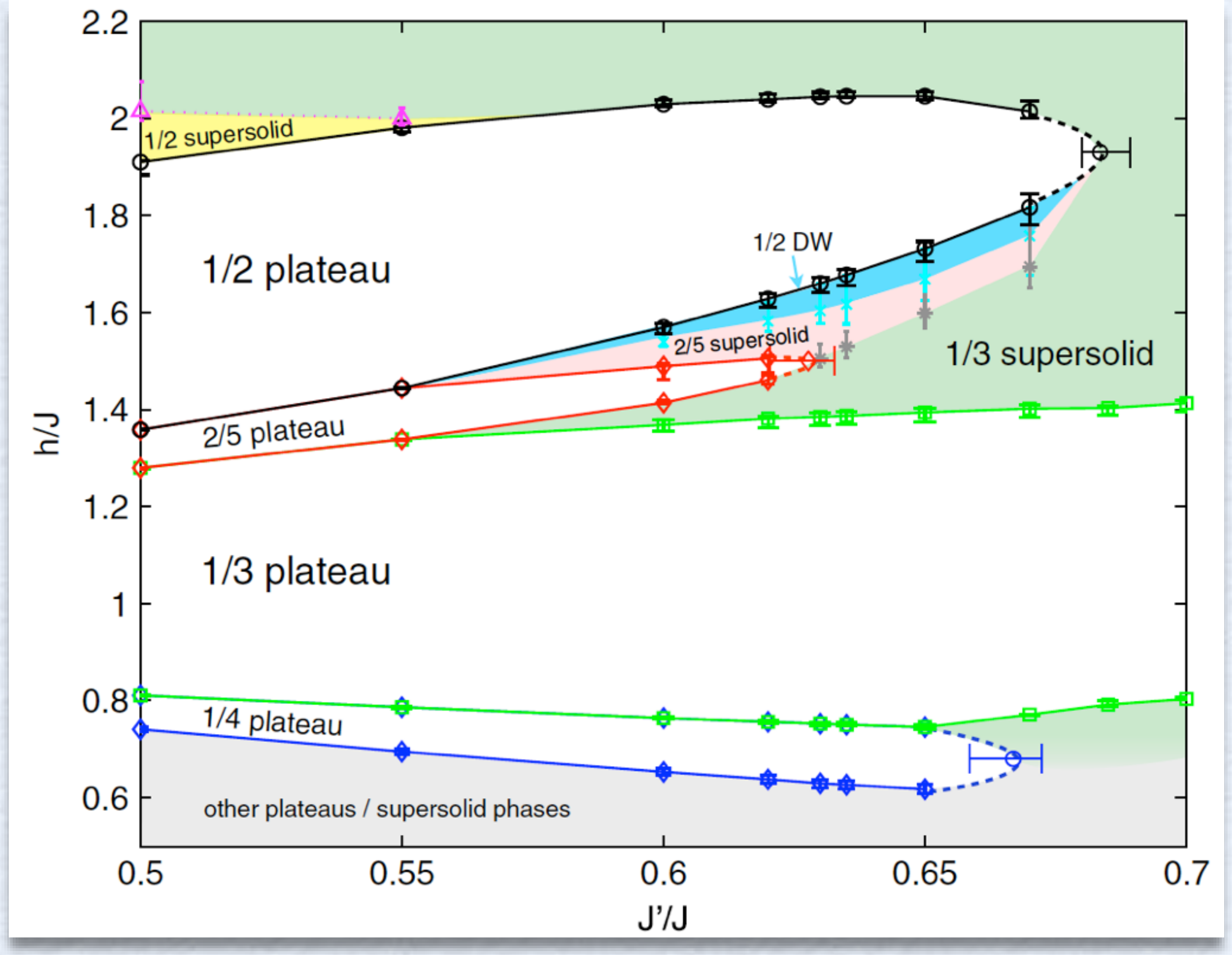


E/N = -0.319179928025625

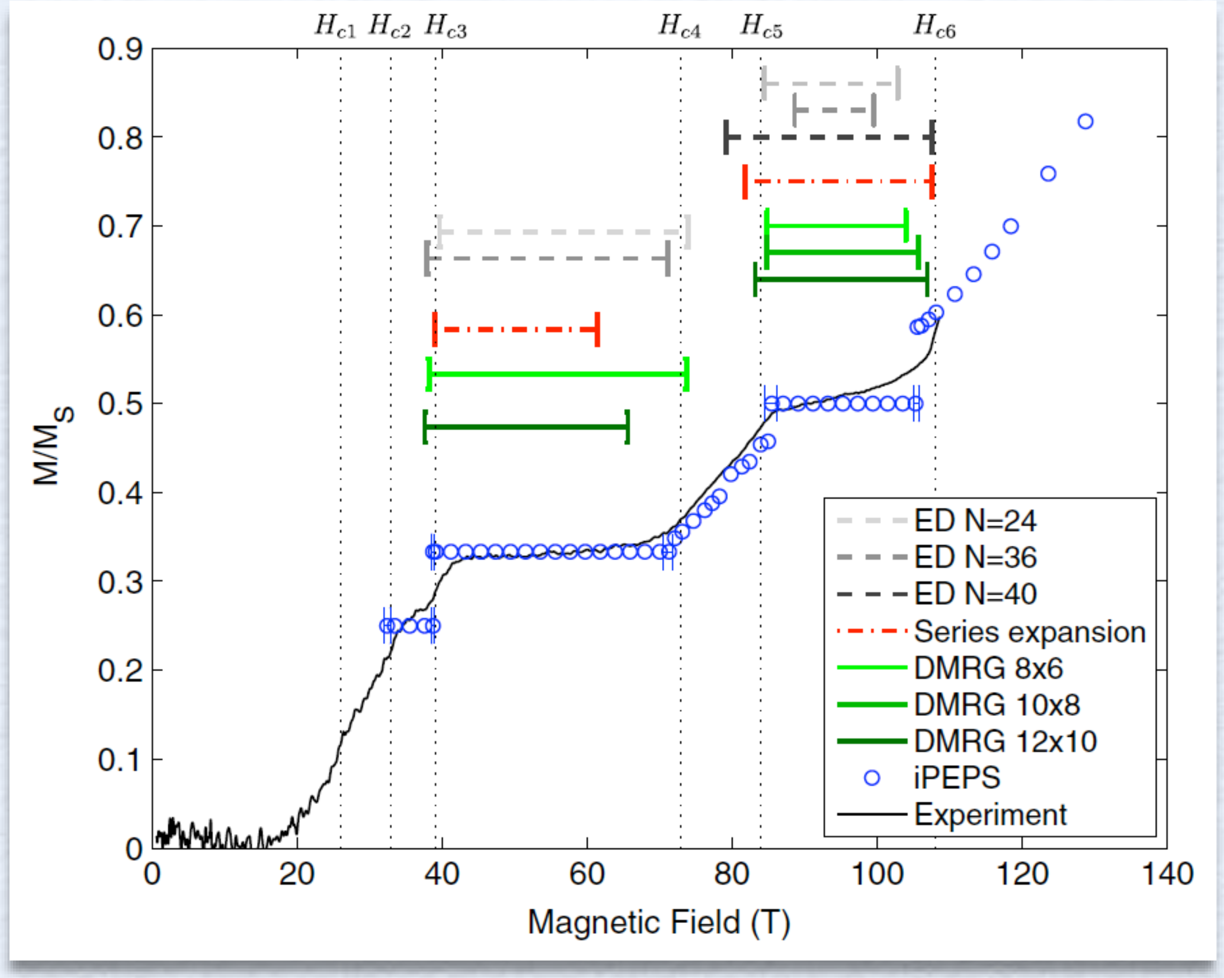
Difference in E/N: only 6e-5 !!!
[S. White on Kagome: difference between VBC and spin-liquid ≈ 1e-3]

Approaching the 2D Shastry-Sutherland lattice: magnetization curve & comparison to experiments

iPEPS (2D, thermod. limit)



J'/J = 0.63:



[Y.H. Matsuda, N. Abe, S. Takeyama, H. Kageyama,
P. Corboz, A. Honecker, S.R. Manmana, G.R. Foltin, K.P. Schmidt, and F. Mila, PRL **111**, 137204 (2013)]

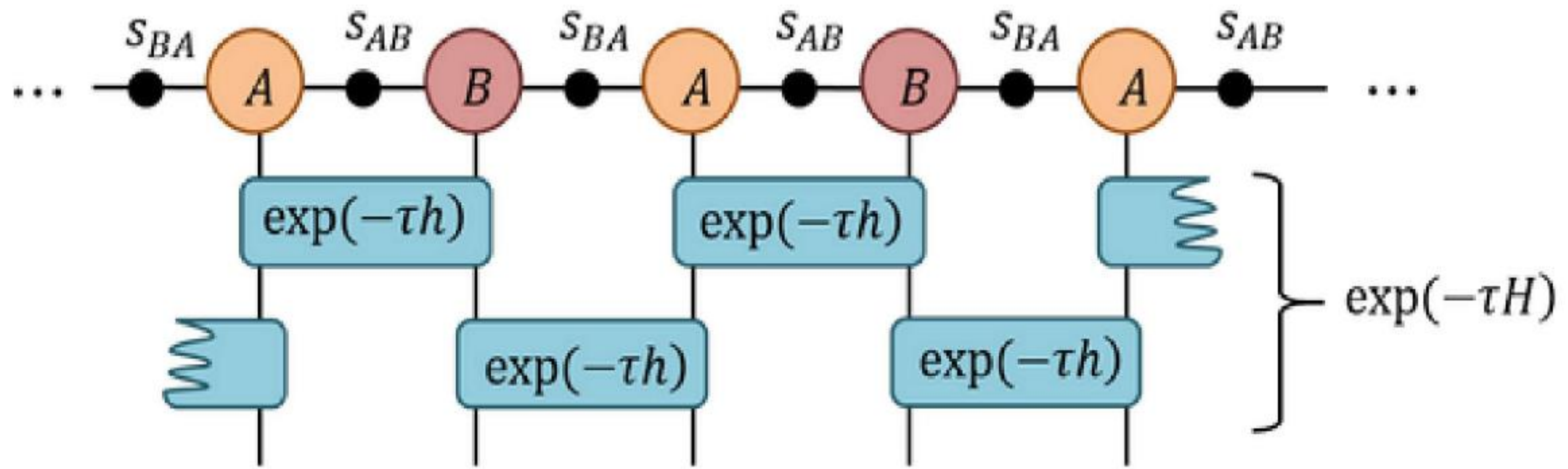
ED & DMRG for Real Time Evolution

Time evolution with Matrix Product States: Trotter approach

Trotter decomposition:

$$e^{-i\,dt\,\hat{H}/\hbar} = \prod_{i\,\mathrm{odd}} e^{-i\,dt\,\hat{H}_i/\hbar} \prod_{i\,\mathrm{even}} e^{-i\,dt\,\hat{H}_i/\hbar} + \mathcal{O}(dt^2)$$

Example: imaginary time evolution („iTEBD“-variant)



[Glen Evenbly, https://www.tensors.net]

Time evolution with Matrix Product States: Krylov-approach

Recall Lanczos projection:
(Krylov-space approach)

$$e^{-i\Delta\tau/\hbar\,\hat{H}}\,|\psi(\tau)\rangle \approx \mathbf{V}_n(\tau)\; e^{-i\Delta\tau/\hbar\,\mathbf{T}_n(\tau)}\;\mathbf{V}_n^{+}(\tau)\,|\psi(\tau)\rangle$$

$$|v_{n+1}\rangle \quad = \quad \mathcal{H}\,|v_n\rangle - a_n\,|v_n\rangle - b_n^2\,|v_{n-1}\rangle$$

$$a_n = \frac{\langle v_n|\,\mathcal{H}\,|v_n\rangle}{\langle v_n|v_n\rangle}\,, \qquad b_{n+1}^2 = \frac{\langle v_{n+1}|v_{n+1}\rangle}{\langle v_n|v_n\rangle}\,, \qquad b_0 = 0$$

Very versatile: arbitrary range interactions & geometries

Two variants:

- „global Krylov method“:
  does not take into account MPS structure – costly!!!
- „local Krylov method“:
  Lanczos-projection while ‚sweeping‘ & sequentely update A-matrices

Time evolution with Matrix Product States: MPO-WI & WII approach

[M. Zaletel et al, PRB **91**, 165112 (2015)]

MPO based time evolution

- Hamiltonian expressed as a sum of terms $\quad H = \sum_x H_x$

Expand $U = \exp(-itH)$ for $t \ll 1$

$$\underbrace{1 + t\sum_x H_x}_{\epsilon \sim \underline{L^2} t^2} \to \underbrace{\prod_x (1 + tH_x)}_{\epsilon \sim \underline{L} t^2}$$

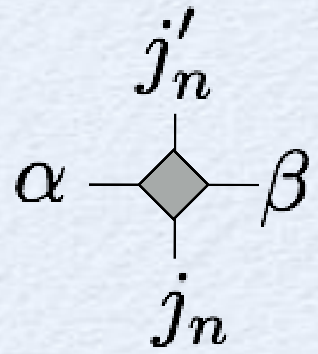
Neglect overlapping terms in expansion

$$\approx 1 + t\sum_x H_x + t^2 \sum_{x<y} H_x H_y$$

$$+ t^3 \sum_{x<y<z} H_x H_y H_z + \dots$$

Compact matrix product operator representation

$$W^{[n] j_n j'_n}_{\alpha\beta} =$$



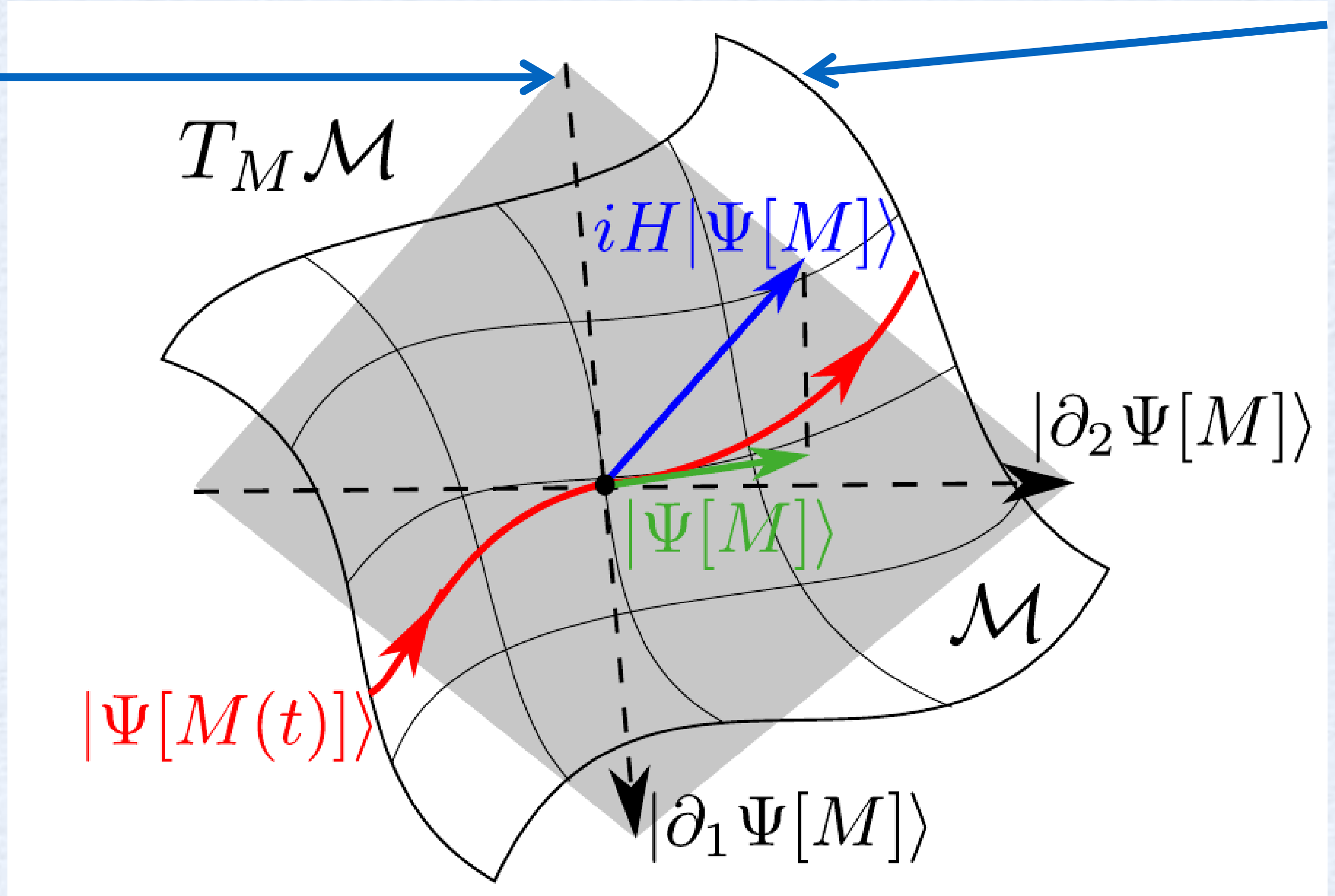
Time evolution with Matrix Product States: Time-dependent variational principle

[J. Haegeman et al, arXiv:1408.5056]

Basic idea of TDVP:

Tangent space

Manifold of MPS states

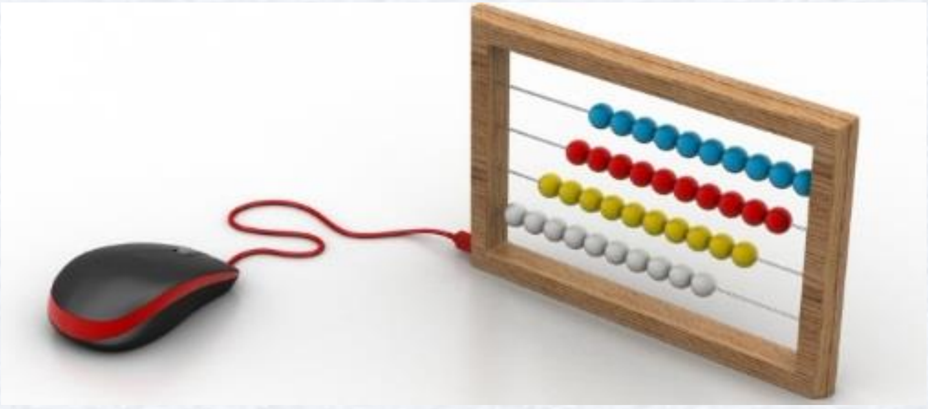


Projection onto tangent Space to MPS manifold:

$$\frac{\mathrm{d}|\Psi[M]\rangle}{\mathrm{d}t} = -iP_{T_{|\Psi[M]\rangle}\mathcal{M}_{\mathrm{MPS}}} H|\Psi[M]\rangle$$

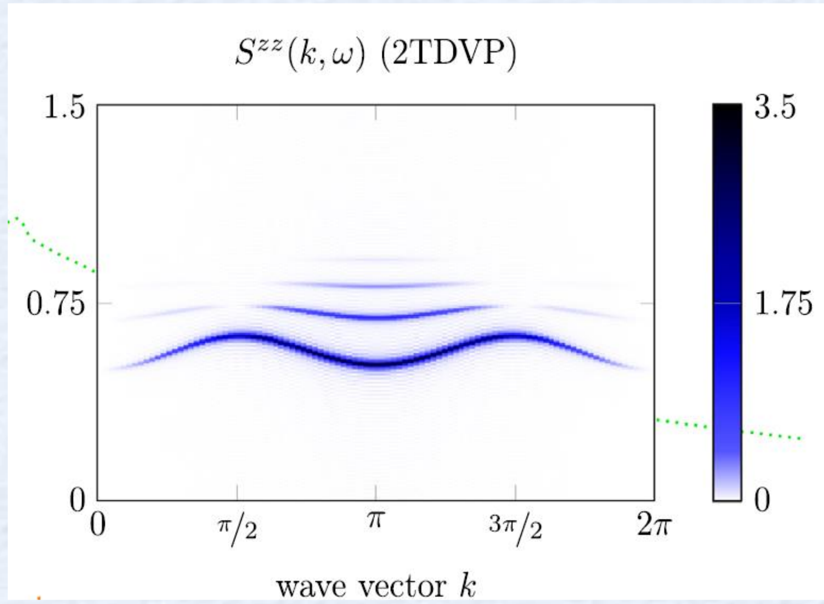
Corrects/improves „local Krylov“ method

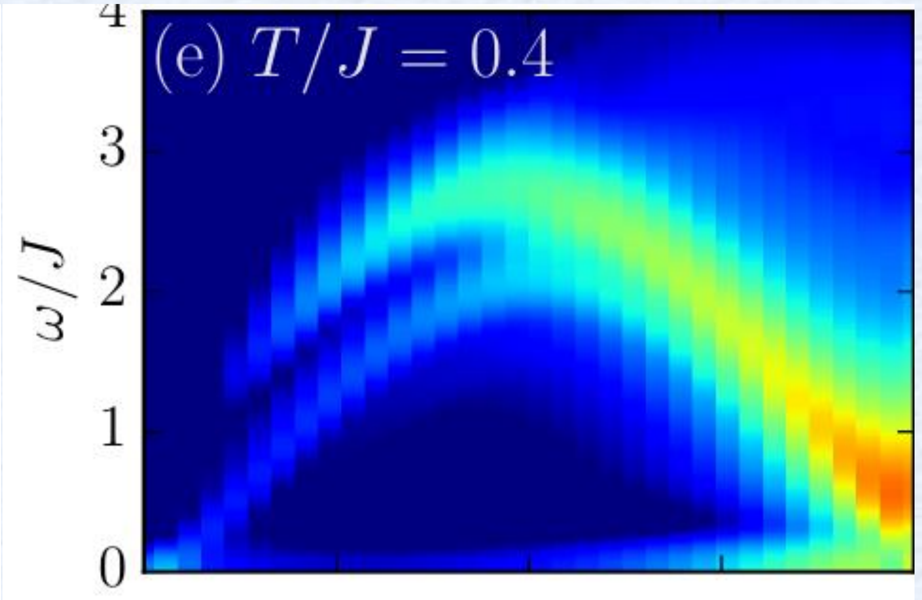
Part III: Dynamics
Spectral Functions and Full Time Evolution



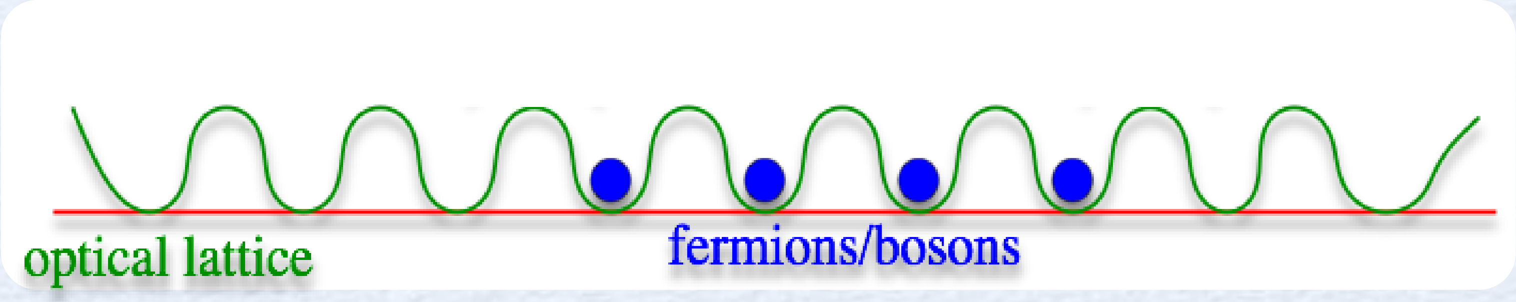
Examples

Dynamical spectral functions (also finite T, nonequilibrium)

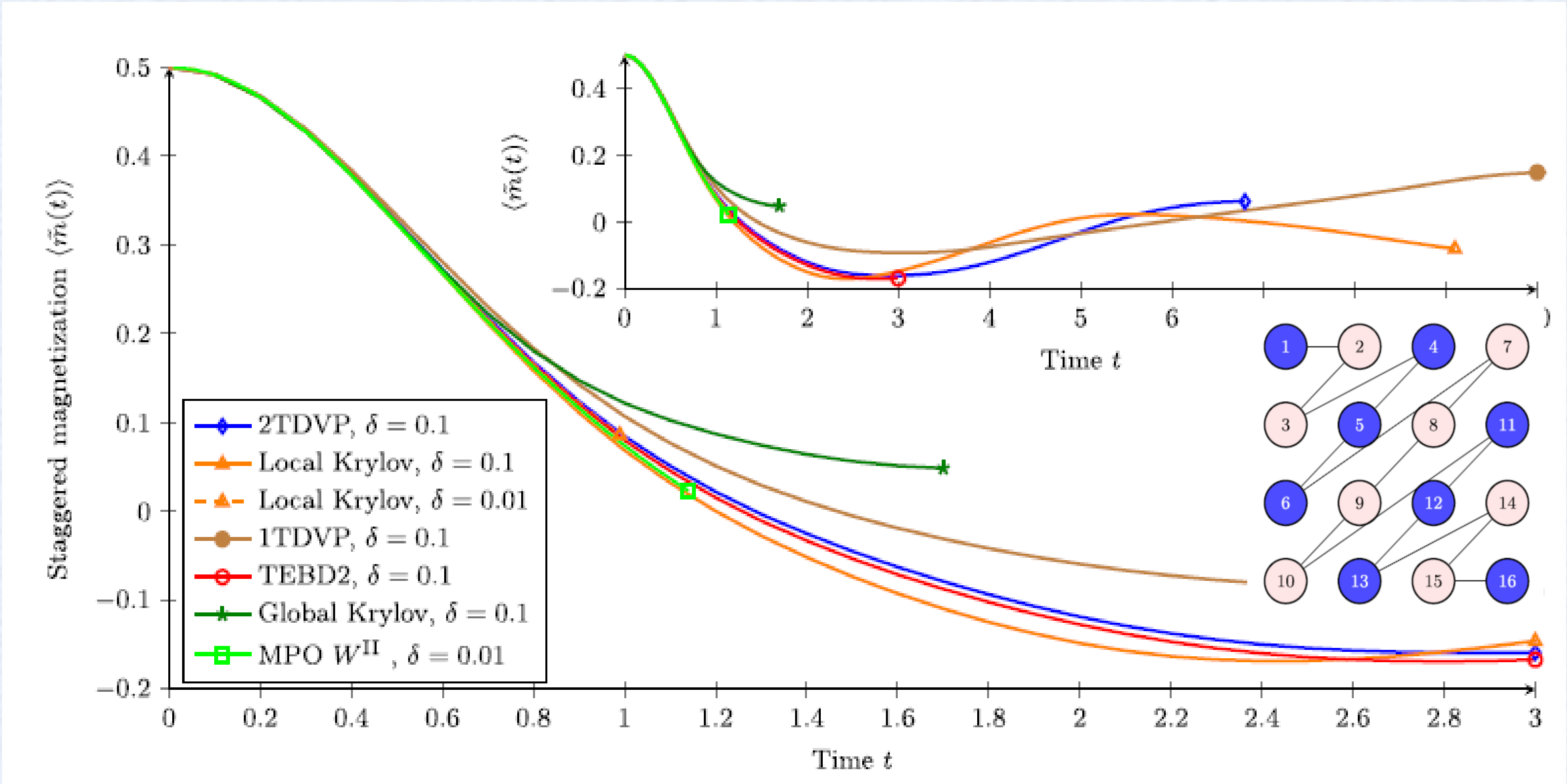




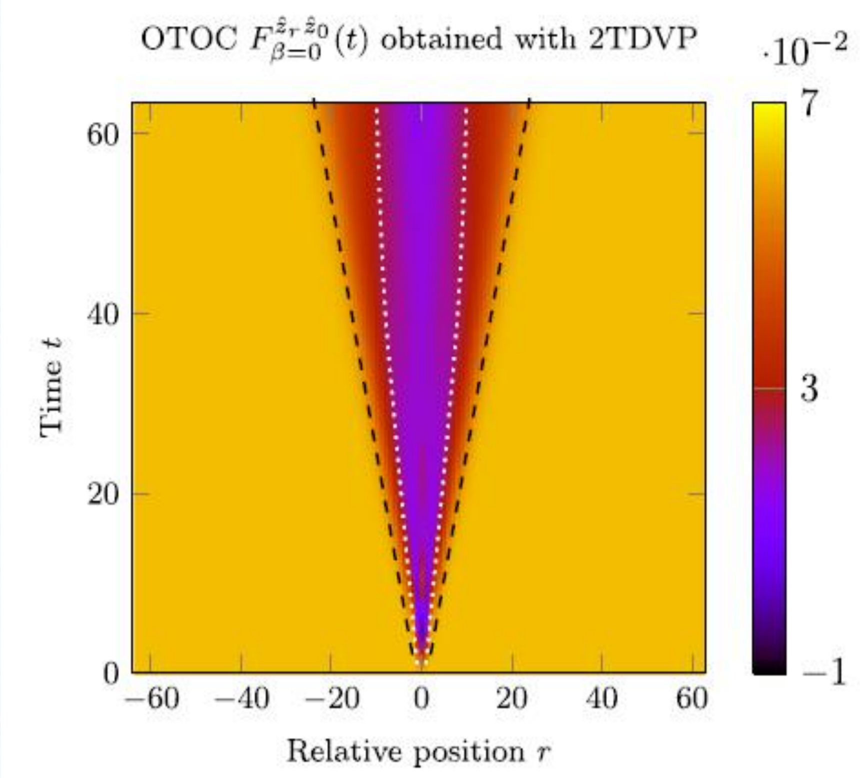
Quantum Quenches (simulate cold gases experiments)

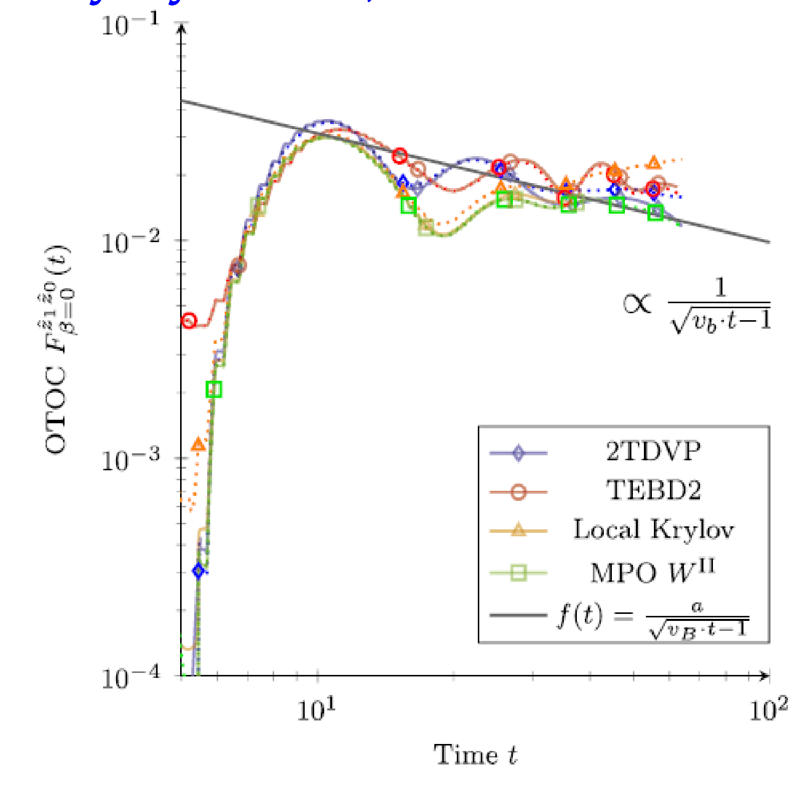


Two-dimensional systems (this is a challenge!!!)



Out-of-time-order, OTOCs
(chaos in quantum many body systems)



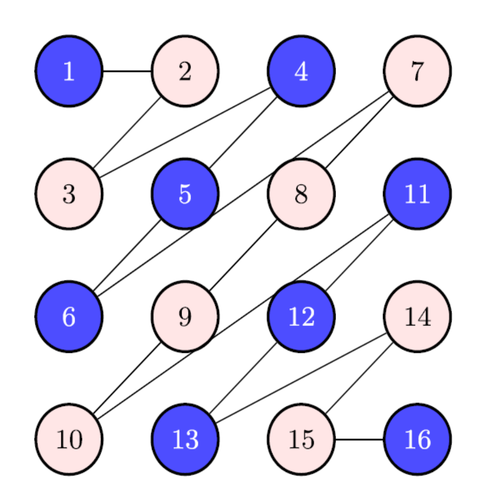


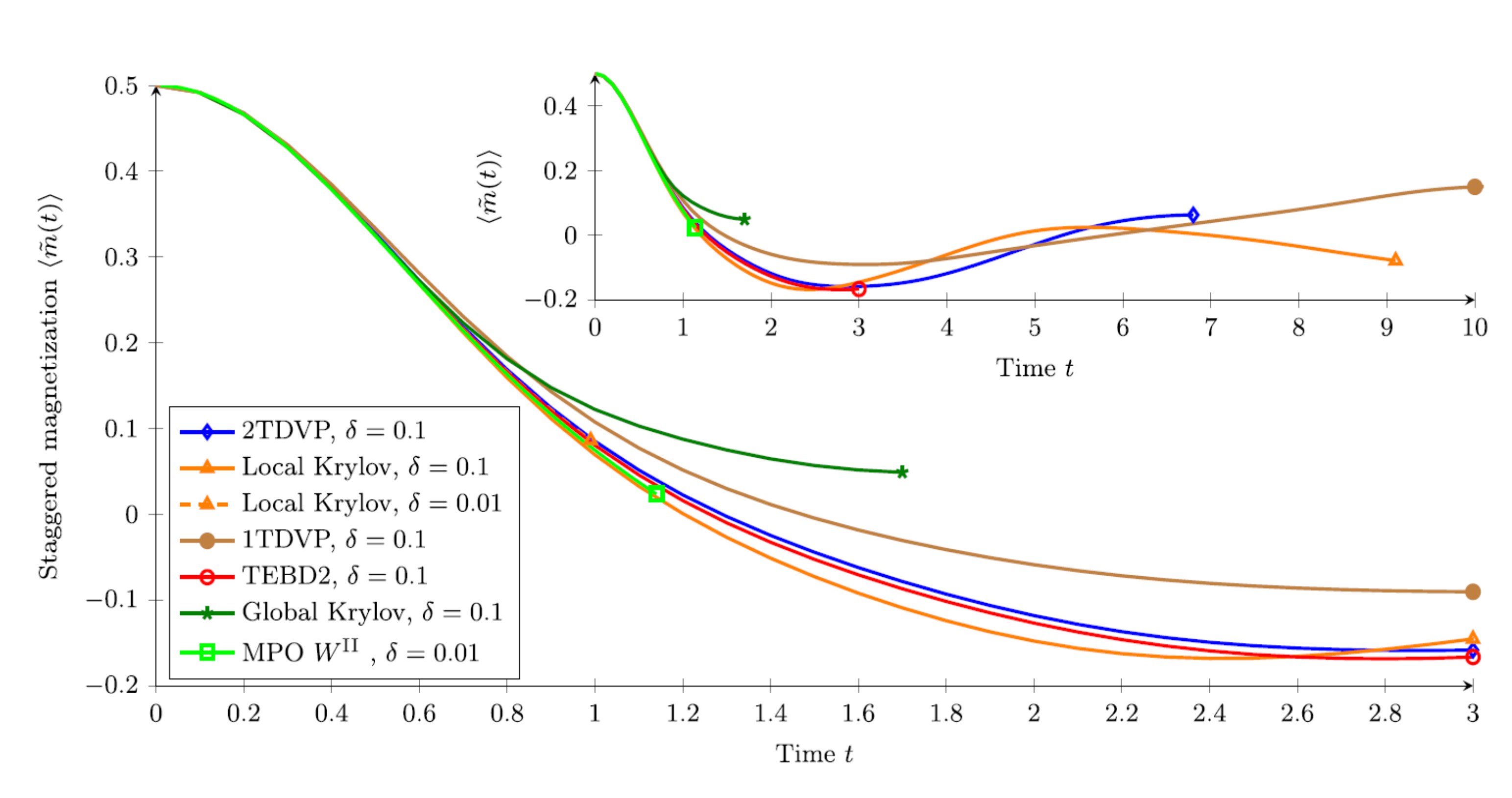
Today's Frontier: Time evolution in two dimensions?

Heisenberg-antiferromagnet,
Neél initial state (product state):

$$\hat{H} = -\sum_{\langle i,j\rangle} \frac{1}{2}\left(\hat{s}_i^+\hat{s}_j^- + \hat{s}_j^+\hat{s}_i^-\right) + \hat{s}_i^z\hat{s}_j^z$$

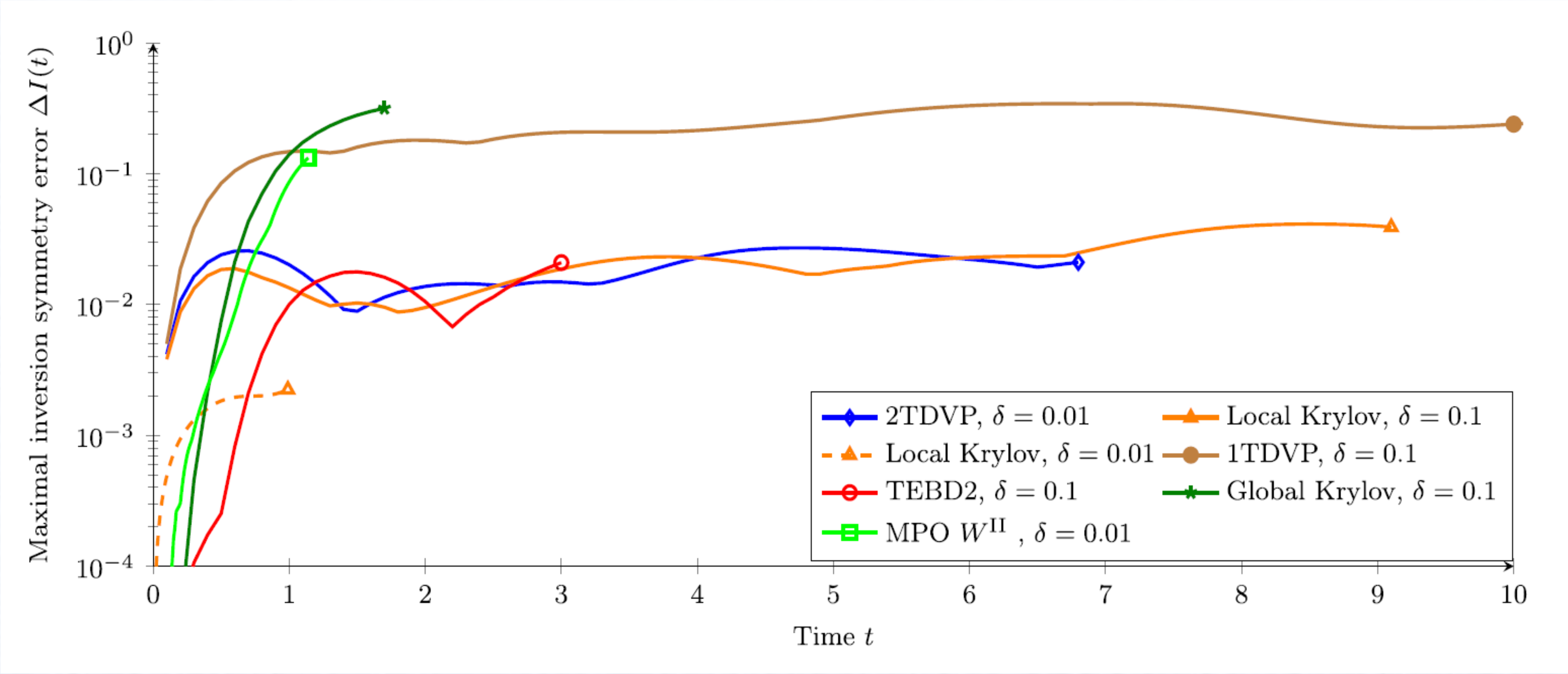
$$|\psi(0)\rangle = \bigotimes_{i\in A}|\downarrow\rangle_i \bigotimes_{j\in B}|\uparrow\rangle_j$$





Fixed bond-dimension m=200:

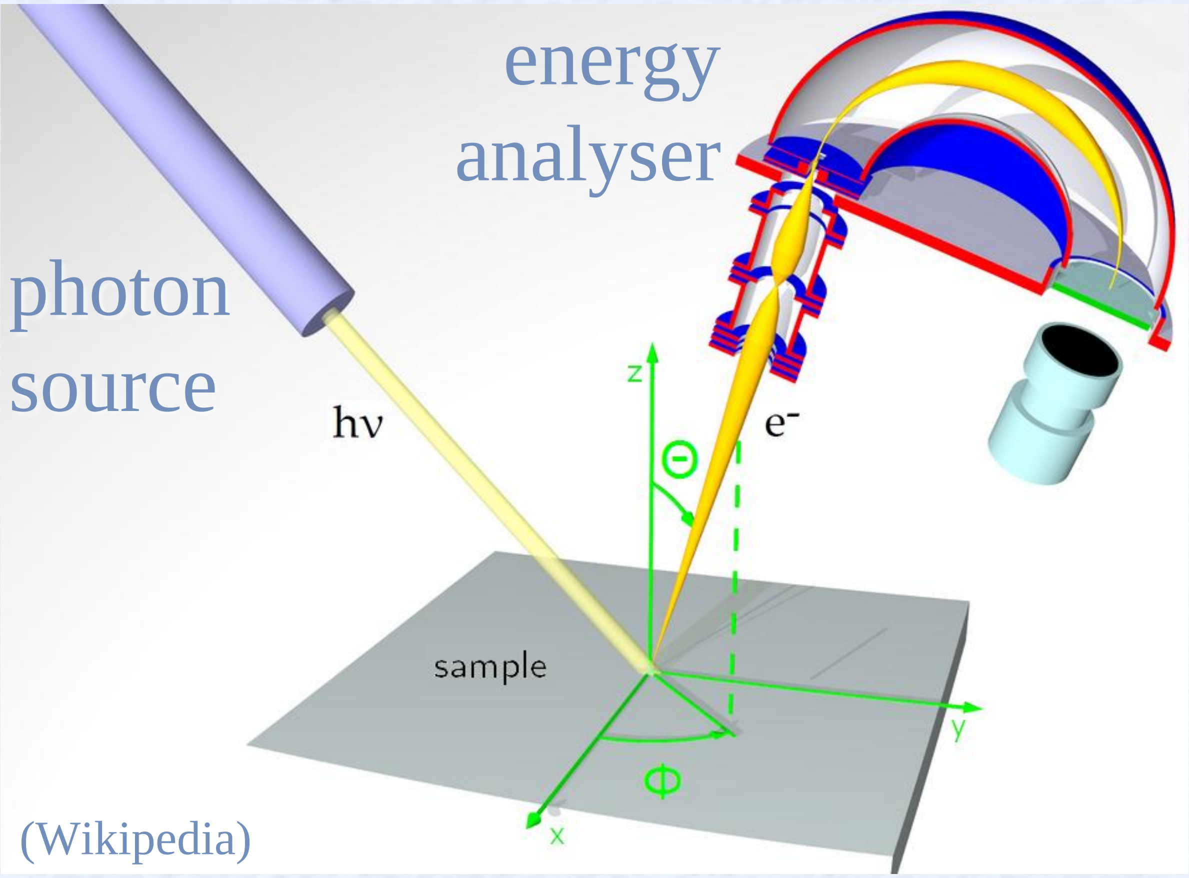
Errors grow rapidly, but some methods perform better than others at short times



Linear Response Dynamics at T=0

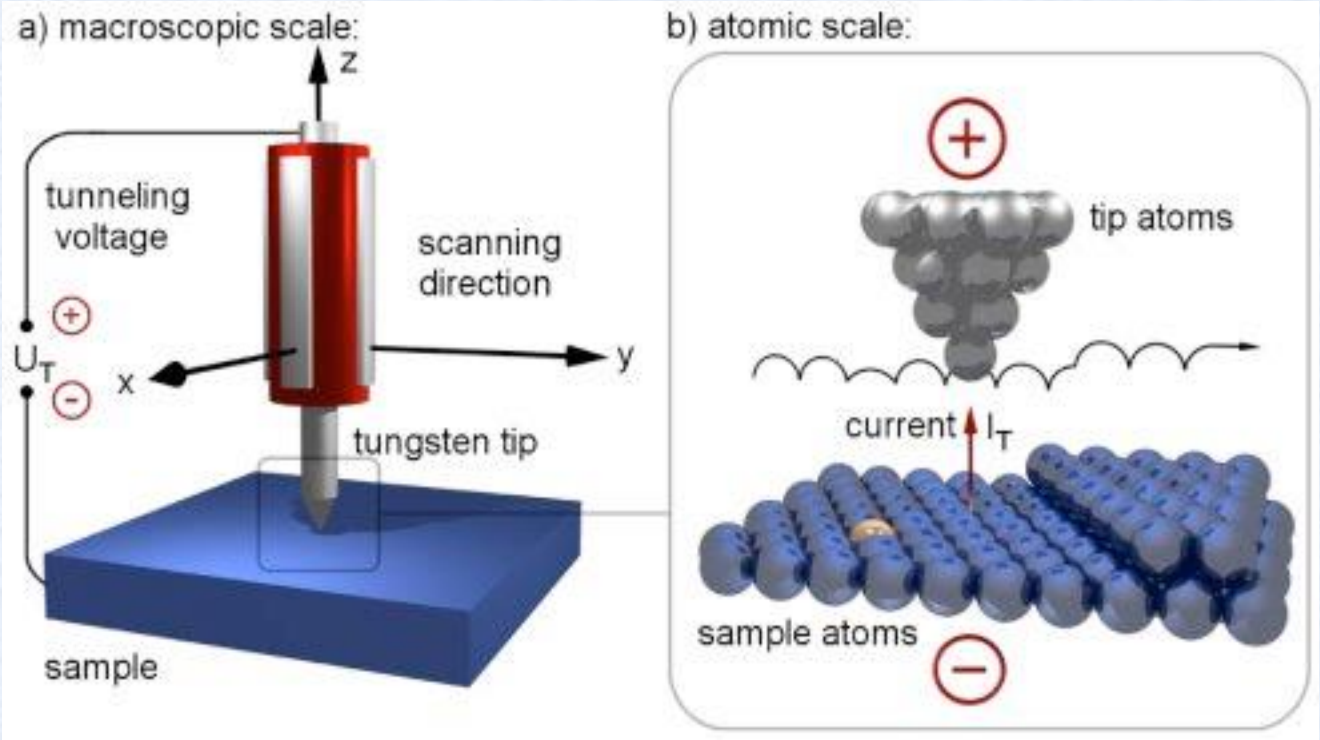
Characterize Many-Body Systems: Dynamical Spectral Functions

angle-resolved photoemission (ARPES)



(Wikipedia)

scanning-tunneling spectroscopy



(www.physics.rutgers.edu/bartgroup/)

Linear response: measure quantities of type:

$$C_{B^\dagger,A}(\omega) \equiv \sum_n \langle\Psi_0|B|n\rangle\,\langle n|A|\Psi_0\rangle\,\delta(\omega-(E_n-E_0))$$

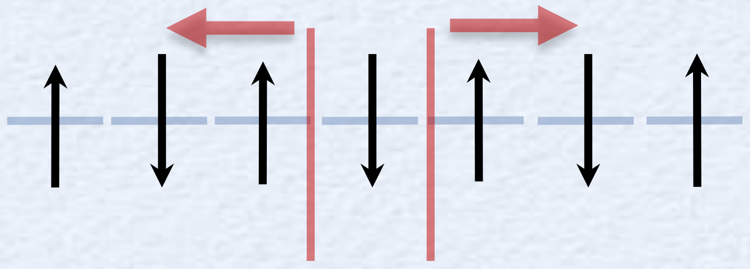
➠ insights into (local) density of states, excitations of the system, structure factors

Linear Response: Spectral Functions at Finite Field

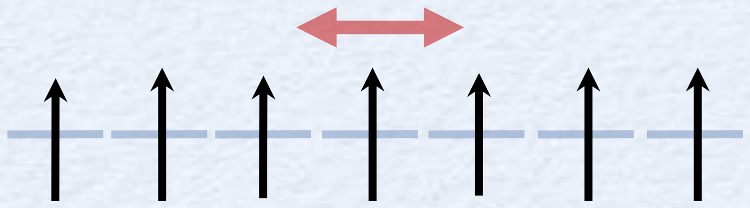
Dynamical structure factor $S^z(k,\omega)$ of a S-1/2 Heisenberg chain when changing an external magnetic field:

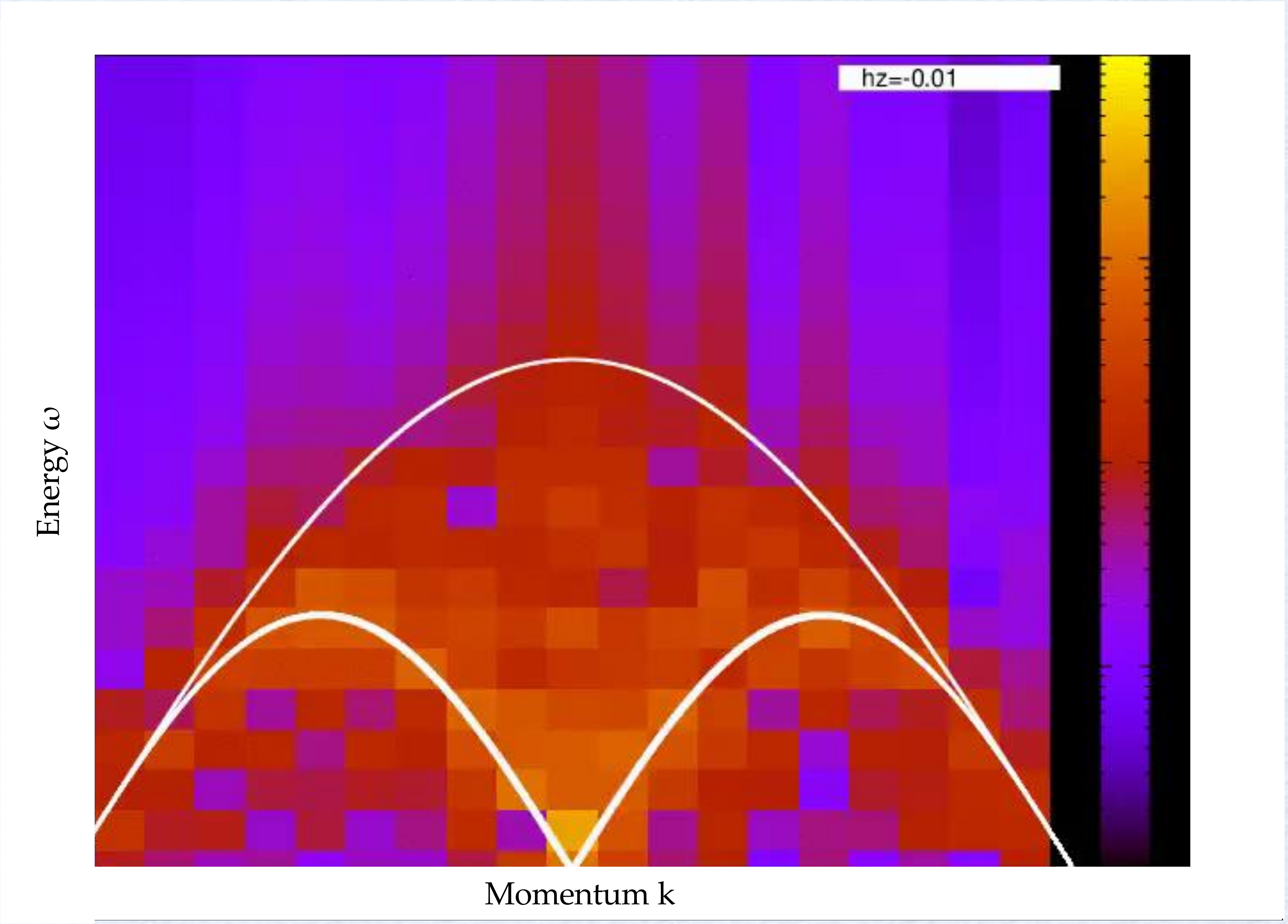
$$\mathcal{H} = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1} - B \sum_i S_i^z$$

small B: spinons



large B: magnons





[T. Köhler, Master thesis, U. Göttingen 2013]

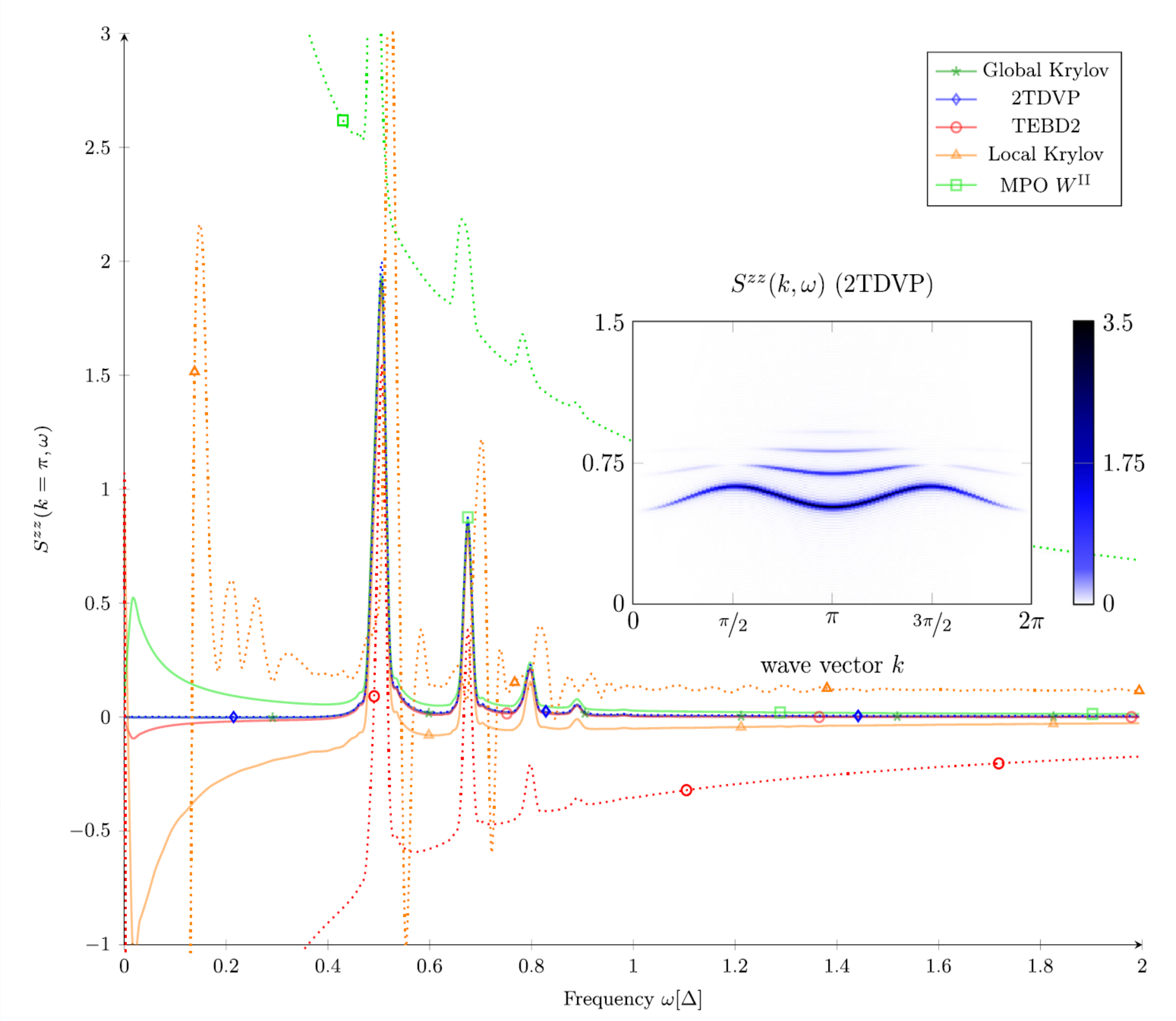
A.C. Tiegel, **S.R.M**. *et al.*, PRB(R) (2014),
A.C. Tiegel *et al.* & **S.R.M.**, PRB (2016),
E.S. Klyushina *et al.*, **S.R.M.**, PRB(R) (2016).

Dynamical correlation functions: Approach using real-time evolution

$$\hat{H} = J\sum_{j=1}^{L}\left[\hat{s}^x_j\hat{s}^x_{j+1} + \hat{s}^y_j\hat{s}^y_{j+1} + \Delta\hat{s}^z_j\hat{s}^z_{j+1} - h^s_j\hat{s}^z_j\right]$$
$$= J\sum_{j=1}^{L}\left[\frac{1}{2}\left(\hat{s}^+_j\hat{s}^-_{j+1} + \hat{s}^-_j\hat{s}^+_{j+1}\right) + \Delta\hat{s}^z_j\hat{s}^z_{j+1} - h^s_j\hat{s}^z_j\right], \quad h^s_j = (-1)^j h$$

$$S^{zz}(q,\omega) = \frac{1}{L}\sum_{j=1}^{L} e^{-iq(j-L/2)}\int_{-\infty}^{\infty} dt\; e^{i\omega t}\,\langle\hat{s}^z_j(t)\hat{s}^z_{L/2}(0)\rangle_{cc}$$
$$\simeq \frac{2\pi}{LT}\delta\sum_{j=1}^{L} e^{-iq(j-L/2)}\sum_{n=0}^{N} e^{i(\omega+i\eta)t_n}\,2\,\mathrm{Re}\,\langle\hat{s}^z_j(t_n)\hat{s}^z_{L/2}(0)\rangle_{cc}$$

Some methods show artifacts at low frequencies – not TDVP



Linear Response Dynamics at $T>0$

Dynamical correlation functions at finite T: Liouvillian formulation

$$G_A(\omega, T) = \frac{1}{Z}\sum_{n,m} e^{-\beta E_m}\langle m|A|n\rangle\langle n|A|m\rangle\delta(\omega-(E_n-E_m))$$

Note: 1) *Difference* of *all* energies

2) MPS approach: $|\Psi_T\rangle$ vector in the Liouville space spanned by $\mathcal{H}_P \otimes \mathcal{H}_Q$

➠ Dynamics is actually governed by Liouville equation [Barnett, Dalton (1987)]

$$\frac{\partial}{\partial t}|\Psi_T\rangle = -i\mathcal{L}|\Psi_T\rangle, \qquad \mathcal{L} = \mathcal{H}_P \otimes I_Q - I_P \otimes H_Q$$

(backward evolution in Q by Karrasch et al.)

$$G_A(k,\omega) = -\tfrac{1}{\pi}\mathrm{Im}\left\langle \Psi_T \middle| A^\dagger \tfrac{1}{z-\mathcal{L}} A \middle| \Psi_T \right\rangle$$

[A.C. Tiegel et al., PRB (2014) : proof of principle calculations]
Earlier: Superoperator approach to mixed-state dynamics [Zwolak & Vidal (2004)]

Liouville space formalism: "Thermofields"

J. Phys. A: Math. Gen. **20** (1987) 411–418. Printed in the UK

Liouville space description of thermofields and their generalisations

S M Barnett† and B J Dalton†‡

† Optics Section, Blackett Laboratory, Imperial College of Science and Technology, London SW7 2BZ, UK
‡ Physics Department, University of Queensland, St Lucia, Queensland, Australia 4067

Received 14 January 1986, in final form 13 May 1986

Abstract. The thermofield representation of a thermal state by a pure-state wavefunction in a doubled Hilbert space is generalised to arbitrary mixed and pure states. We employ a Liouville space formalism to investigate the connection between these generalised thermofield wavefunctions and a generalised thermofield state vector in Liouville space which is valid for all cases of the quantum density operator. The system dynamics in the Schrödinger and Heisenberg pictures are discussed.

+ references therein

$$i\frac{d\varrho}{dt} = \left[\hat{H}, \varrho\right] \Rightarrow i\frac{d}{dt}|\varrho\rangle\rangle = \mathcal{L}|\varrho\rangle\rangle$$

von Neumann equation

Liouville equation

Dynamical correlation functions: Chebyshev recursion

☞ Representation via Chebyshev polynomials:

[MPS: A. Holzner *et al.*, PRB **83**, 195115 (2011); A. Weiße *et al.*, RMP **78**, 275 (2006)]

$$G_A(\omega) = \frac{2}{\pi W \sqrt{1-\omega'^2}} \left[g_0\, \mu_0 + 2 \sum_{n=1}^{N-1} g_n\, \mu_n T_n(\omega') \right]$$

with

$$\mu_n = \langle t_0 | t_n \rangle = \left\langle \Psi_T \left| A^\dagger T_n(\mathcal{L}') A \right| \Psi_T \right\rangle$$

$$\boxed{|t_0\rangle = A|\Psi_T\rangle, \quad |t_1\rangle = \mathcal{L}'|t_0\rangle, \quad |t_n\rangle = 2\mathcal{L}'|t_{n-1}\rangle - |t_{n-2}\rangle}$$

W : bandwidth of $\mathcal{L}$

$\mathcal{L}'$: rescaled Liouvillian, so that $W \to [-1, 1]$

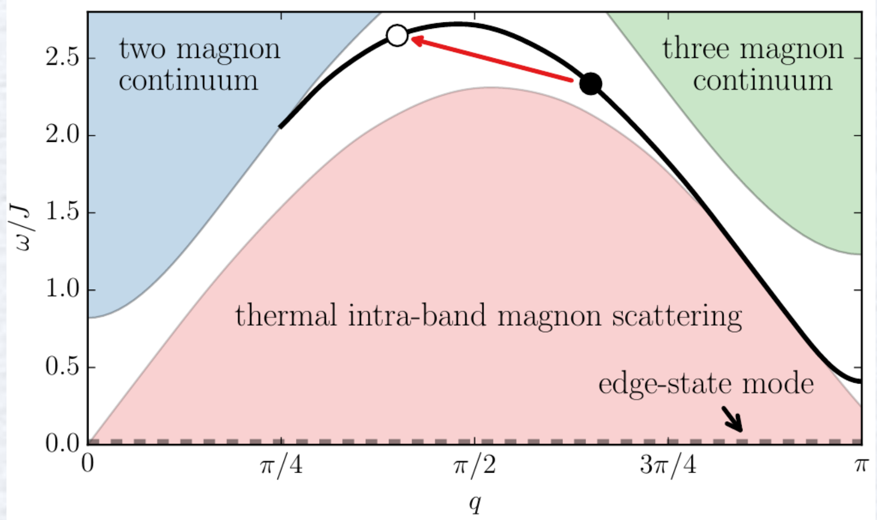
$$\boxed{\omega' \in [-1,1],\, T_n(\omega') = \cos\left[n\left(\arccos \omega'\right)\right]}$$

g_n : damping factors $\rightarrow$ Gaussian broadening $\eta \sim 1/N$

$$g_n^J = \frac{(N-n+1)\cos\frac{\pi n}{N+1} + \sin\frac{\pi n}{N+1}\cot\frac{\pi}{N+1}}{N+1}$$

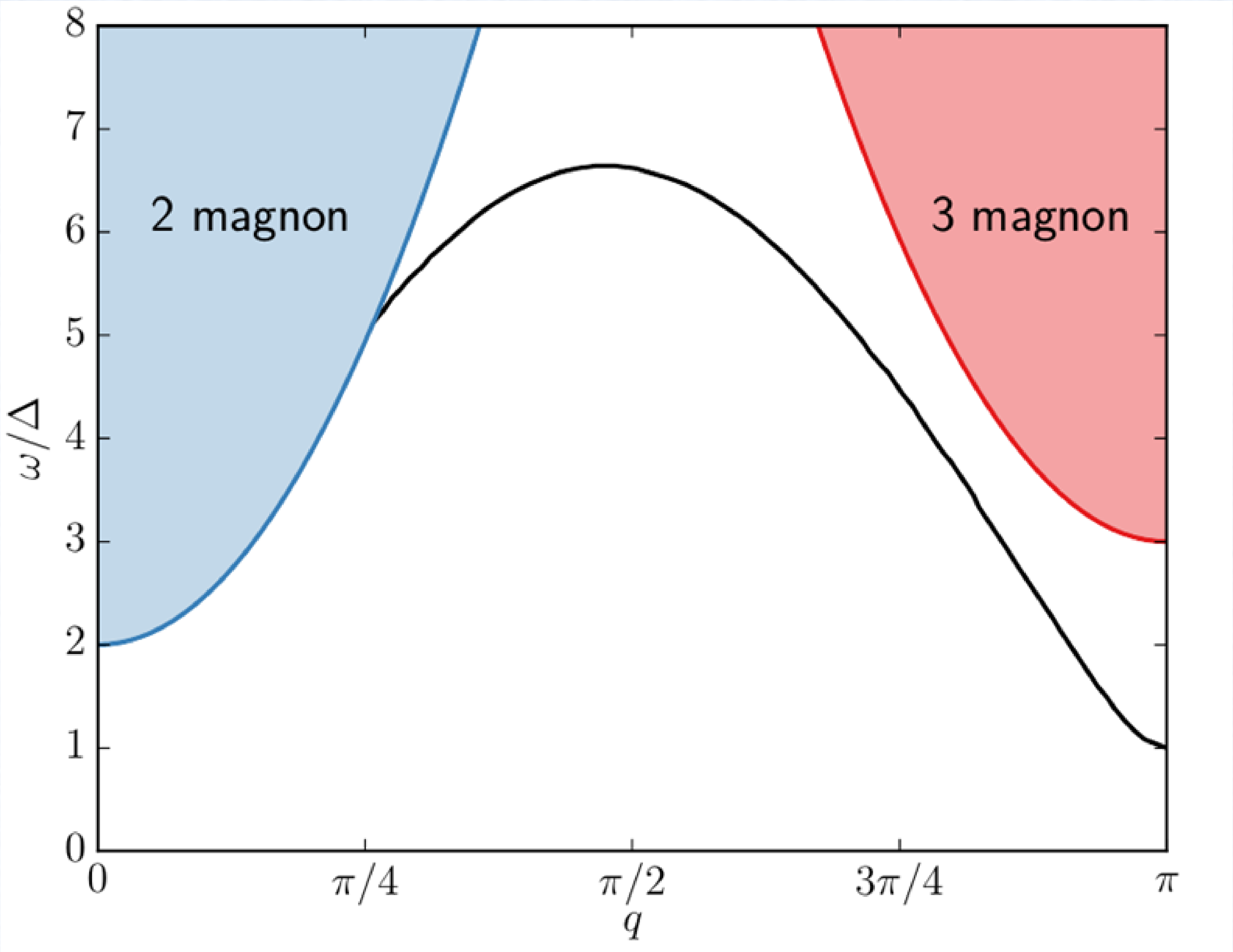
"Jackson damping"

Finite-T dynamics in spin-1 chains



➠ New features in the spectra at T>0?

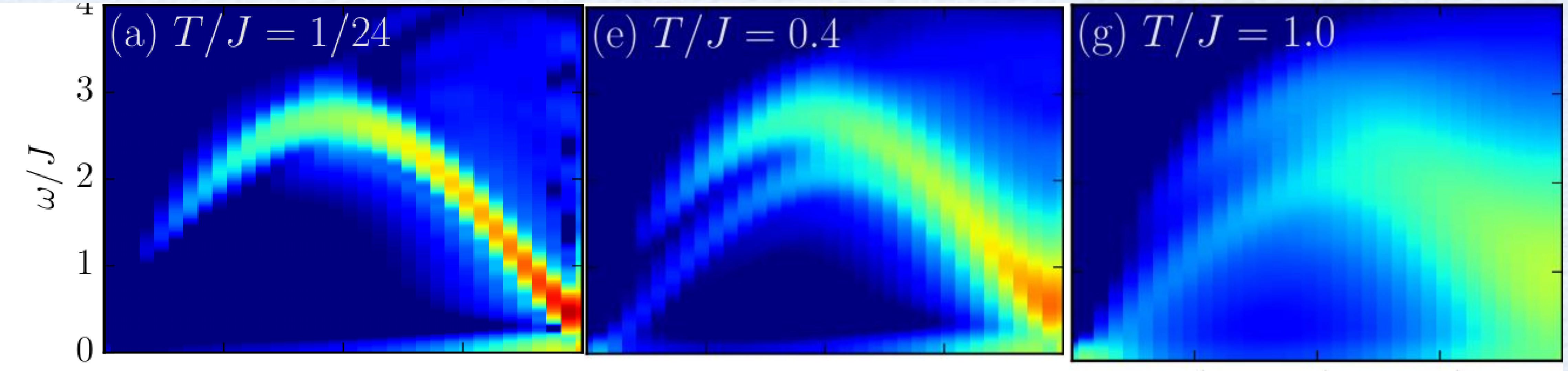
Spin-1 chains: Spectral functions at T=0



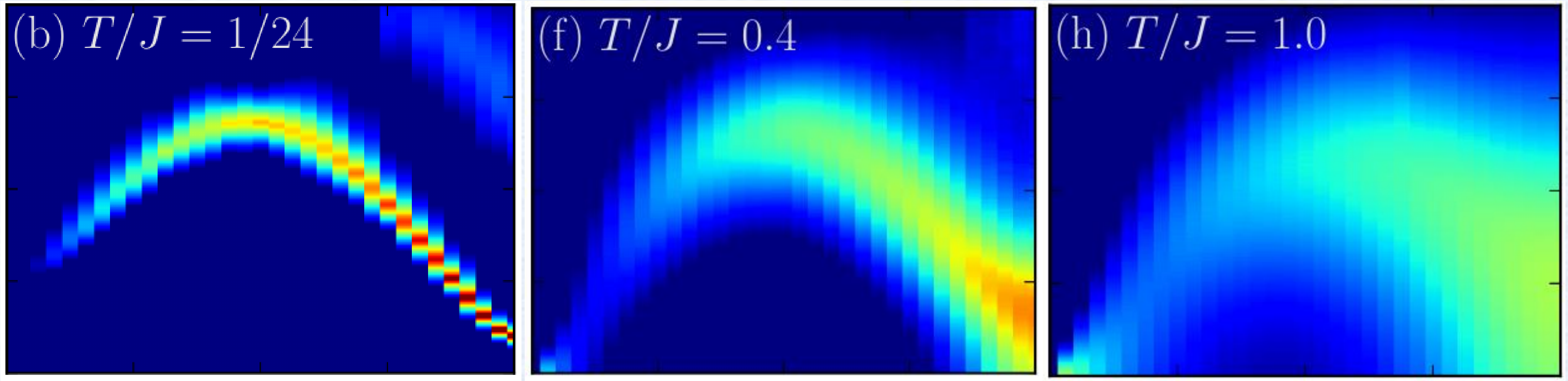
S.R. White & I. Affleck, PRB (2008)

Spin-1 chains:
Spectral functions at T=0 and T>0

DMRG, OBC, L=32:



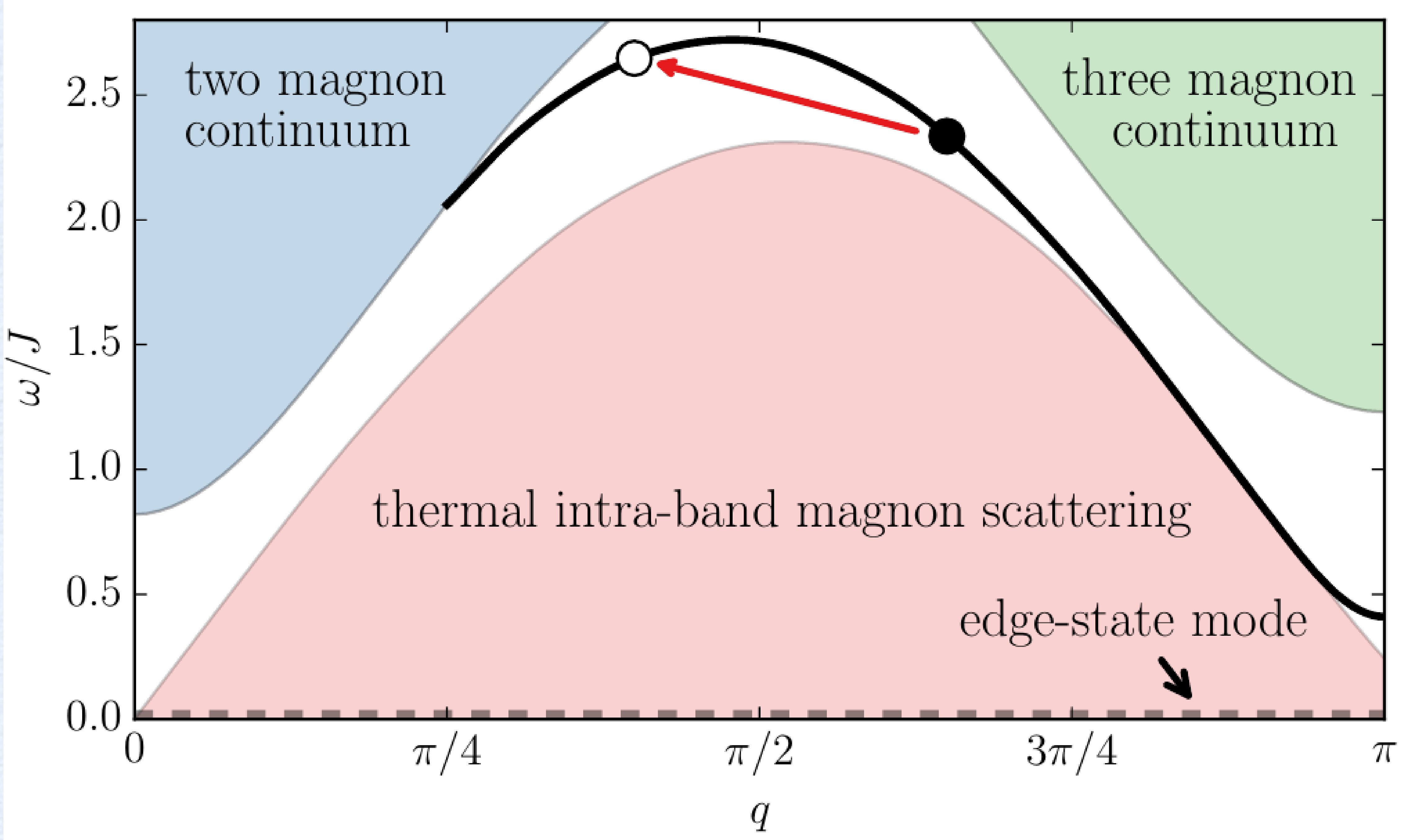
QMC, PBC, L=64:



Two new features:

- At finite T, a new branch appears *below* the magnon branch
  scattering of thermally excited magnons
- With OBC, a signature of the edge-state is obtained, also at T>0

Spin-1 chains: Spectral functions at T>0

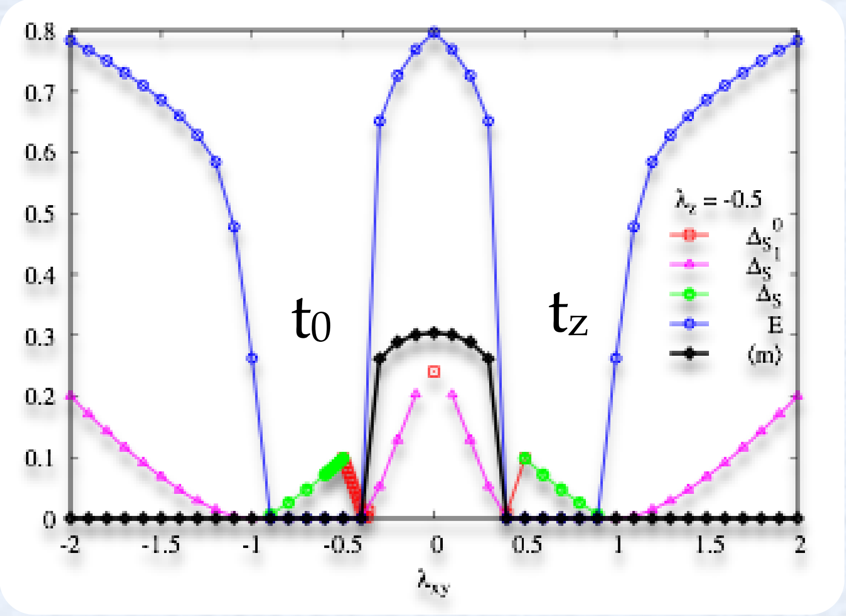


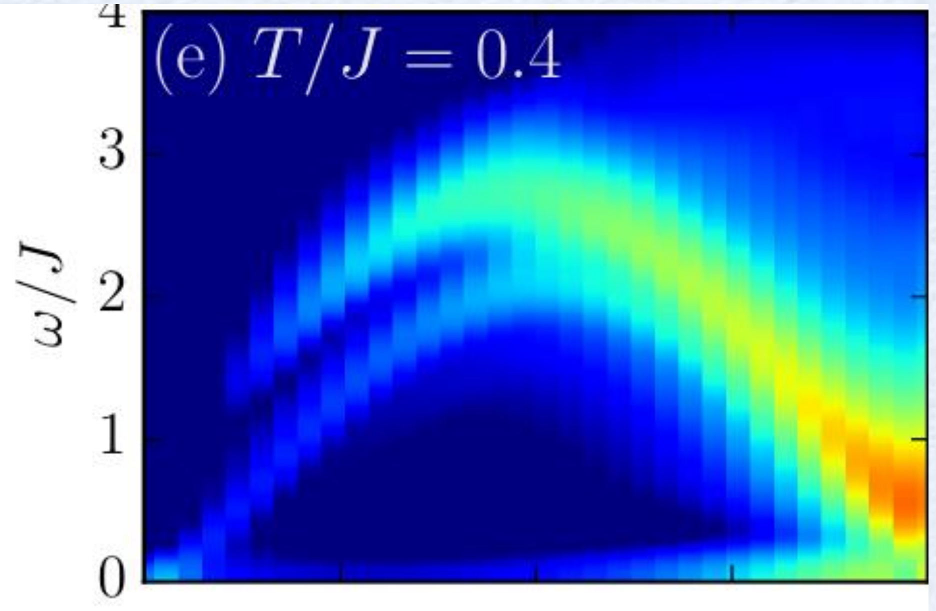
J. Becker, T. Köhler, A.C. Tiegel, S.R. Manmana, S. Wessel, and A. Honecker, PRB **96**, 060403(R) (2017).

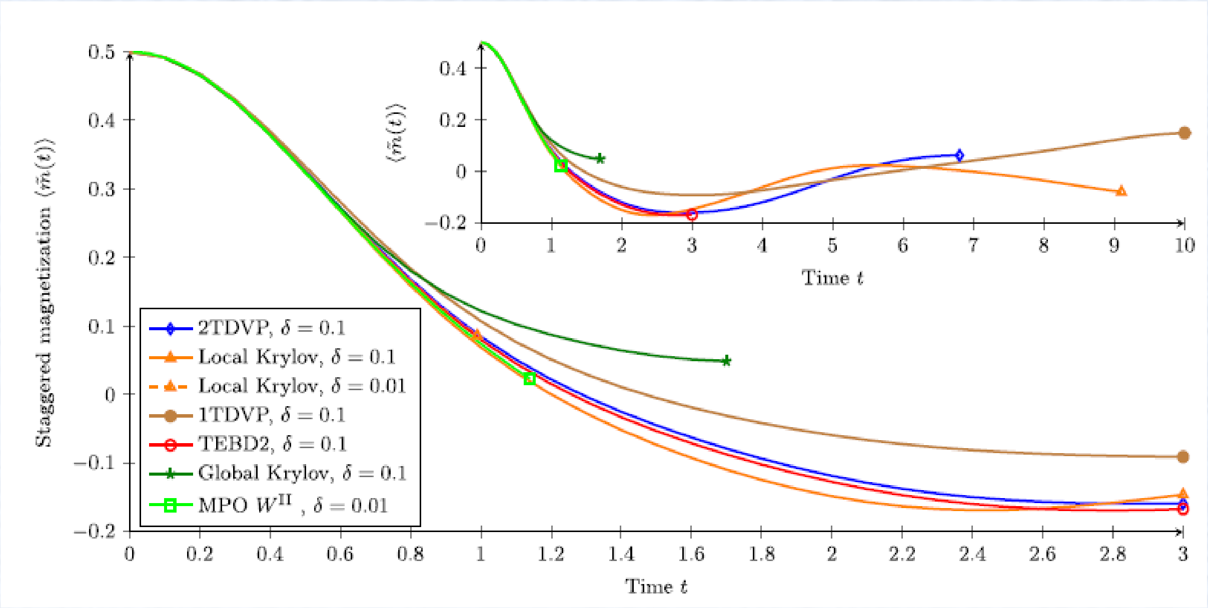
Conclusions & Outlook

Tensor Network methods very flexible and powerful tools:

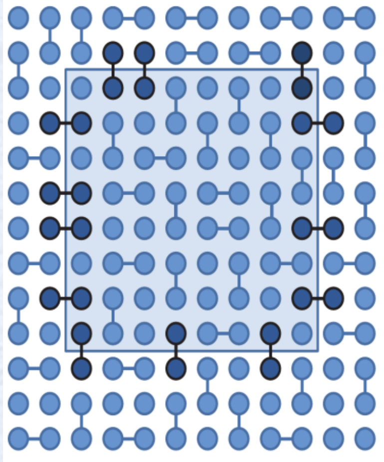
- Basic idea: ‚data compression'
- Ground states, phase diagrams, finite-T, spectral functions, nonequilibrium







- Quantity controling the „quality" of MPS: Entanglement



$$S = -\sum_j w_j^2 \log w_j^2$$

Frontier of today's research: how to deal with the entanglement?