Application of Matrix Product States to Condensed Matter and Ultracold Gases

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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

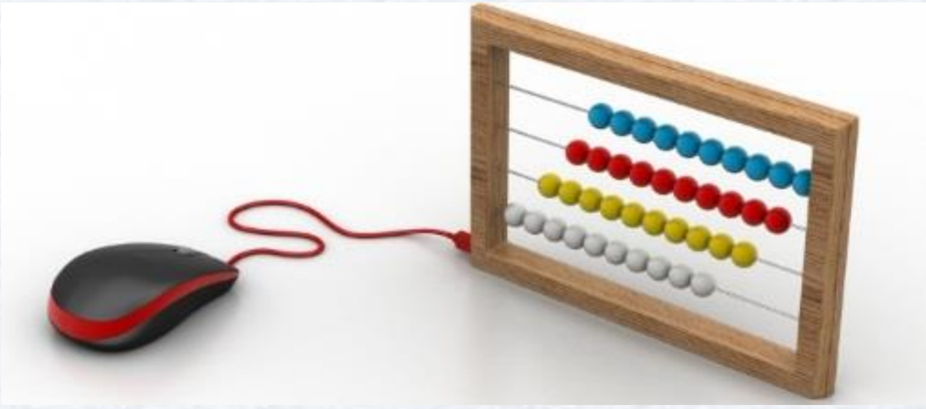
arXiv:cond-mat/0409292,
Rev. Mod. Phys. **77**, 259 (2005)

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)

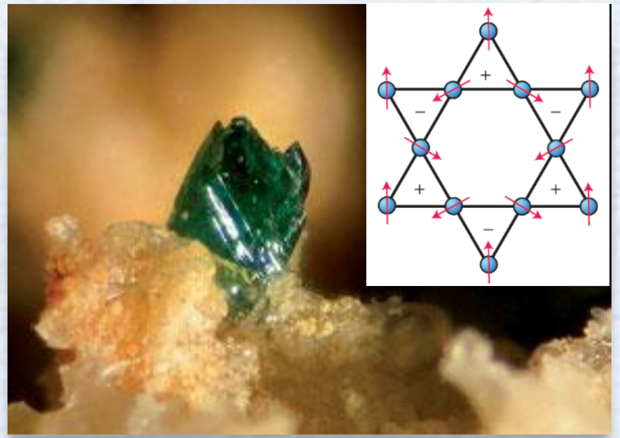
Part I: General Overview



Quantum Many-Body Systems: in Nature and in the Lab

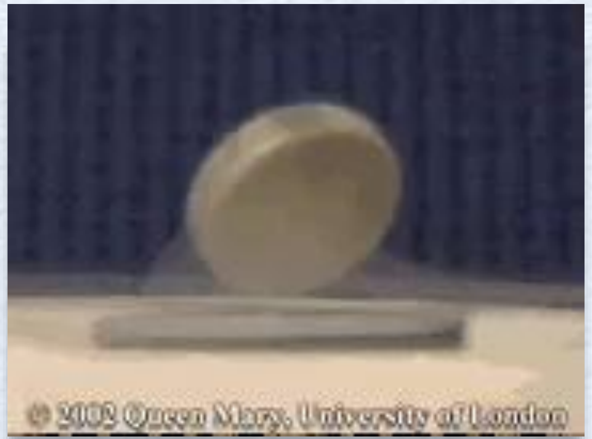
Quantum Magnetism in Natural Minerals

Synthesized Materials: Cuprates



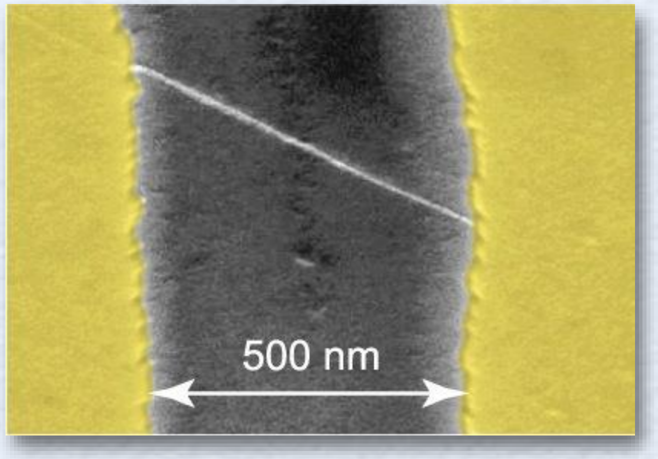
Introduction to Frustrated Magnetism
C. Lacroix, P. Mendels, F. Mila, Springer (2011)

$$\hat{H} = -\sum_i \frac{\hbar^2}{2m_i}\vec{\nabla}_i^2 + \sum_{i\neq j}\hat{V}\left(\vec{x}_i, \vec{x}_j\right)$$



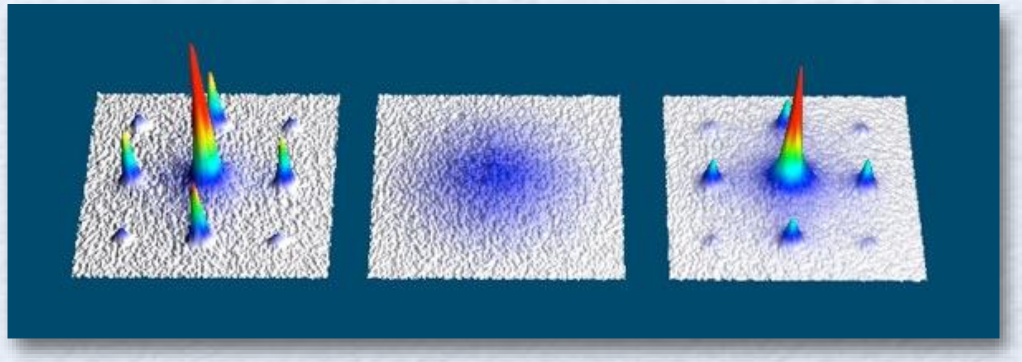
Correlated Electrons in high-temperature superconductors
E. Dagotto, Rev. Mod. Phys. (1994)

Goal: Identify new states of matter



Quantum Physics in One Dimension,
T. Giamarchi, Clarendon Press (2004)

Quantum Wires, Low Dimensions



Many-body physics with ultracold gases
I. Bloch, J. Dalibard & W. Zwerger, Rev. Mod. Phys. (2008)

Ultracold Gases (Optical Lattices)

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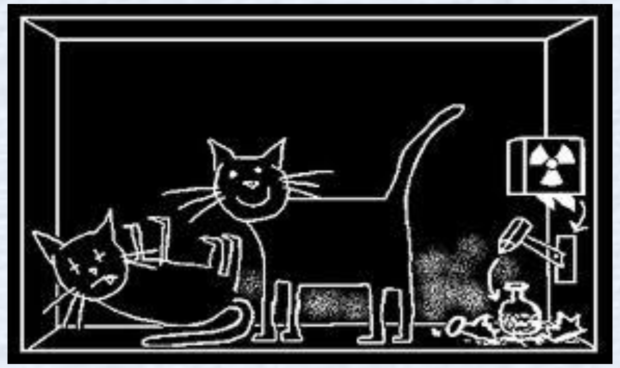
Quantum Many-Body Systems: Superposition & Entanglement

I) Superposition of states is *also* a possible state

$$|\psi\rangle = |\text{dead}\rangle + |\text{alive}\rangle$$



II) Entanglement: spin-1/2 particles (e.g., electrons)

2 particles: 4 possible states

$$|\psi\rangle = \begin{cases} |\uparrow\rangle \otimes |\uparrow\rangle \\ |\uparrow\rangle \otimes |\downarrow\rangle \\ |\downarrow\rangle \otimes |\uparrow\rangle \\ |\downarrow\rangle \otimes |\downarrow\rangle \end{cases}$$

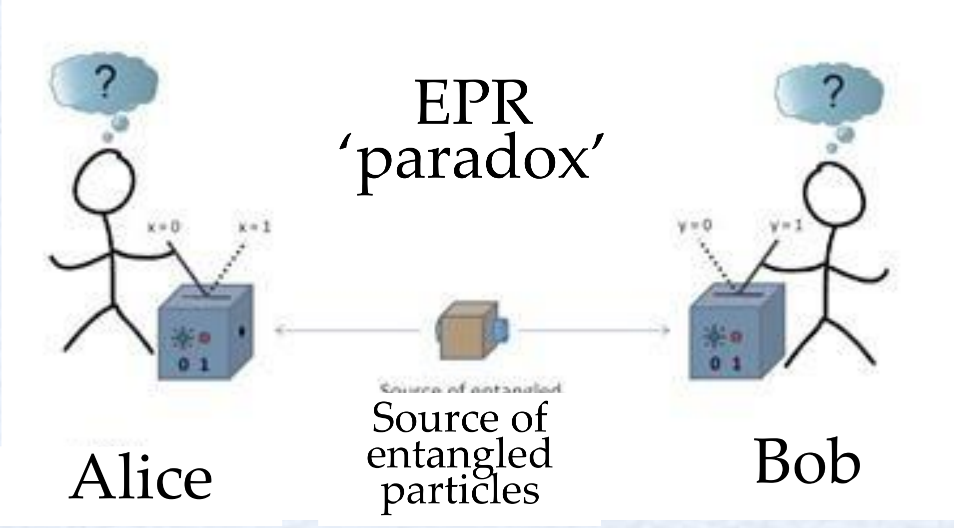
"classical", "product state"

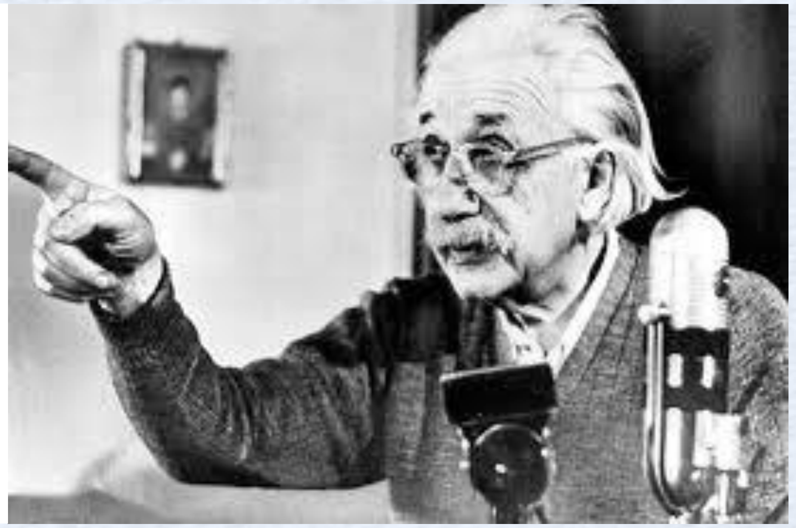
$$\boxed{|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle \otimes |\uparrow\rangle + |\downarrow\rangle \otimes |\downarrow\rangle\right)}$$

"entangled": not a product state

Einstein:

«spooky action at a distance»





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

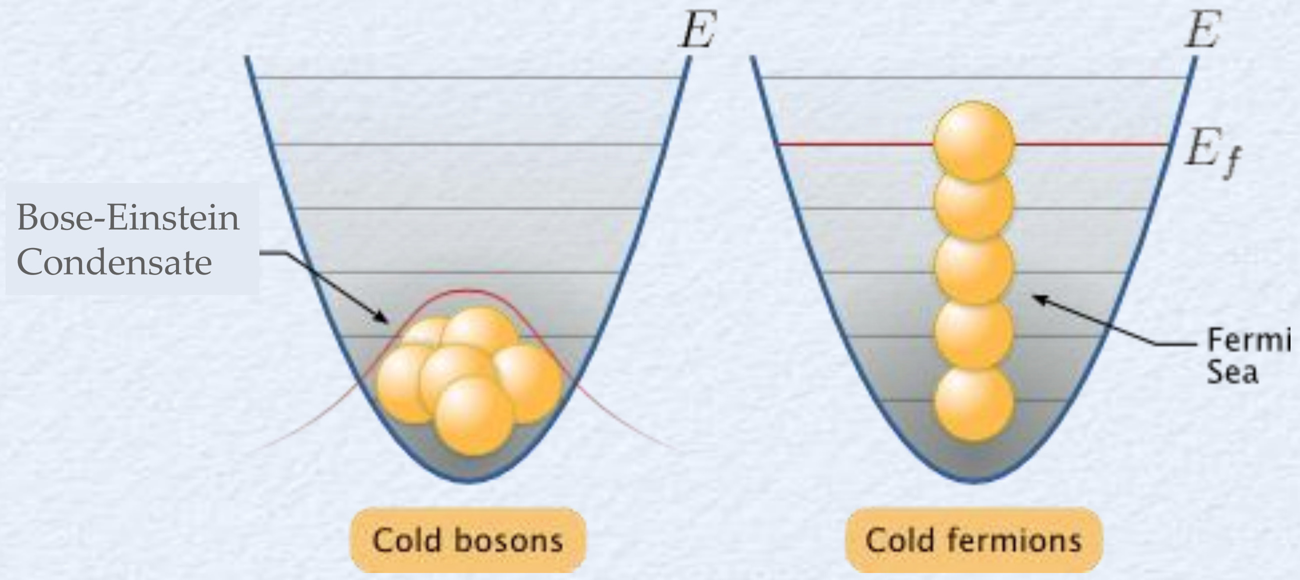
b) because of mutual interactions.

Small numerical values: need *accurate* methods

Quantum Many-Body Systems: Quantum Statistics

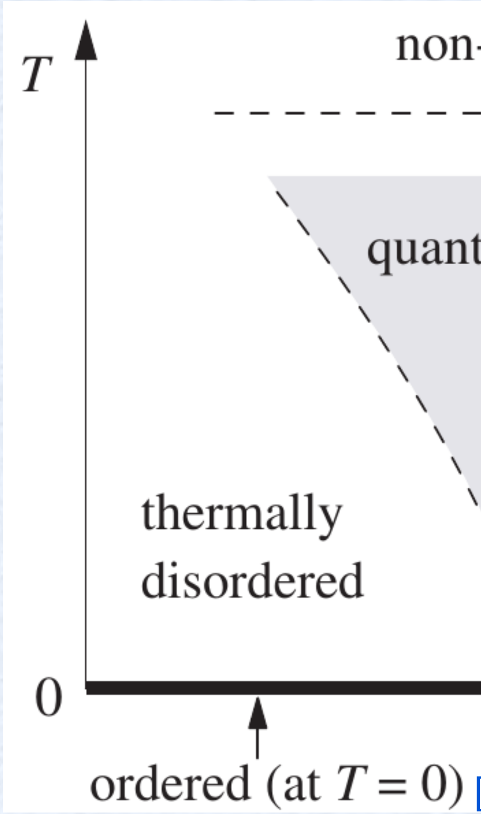
Exchange statistics:

Behavior at low temperatures:



At T=0:

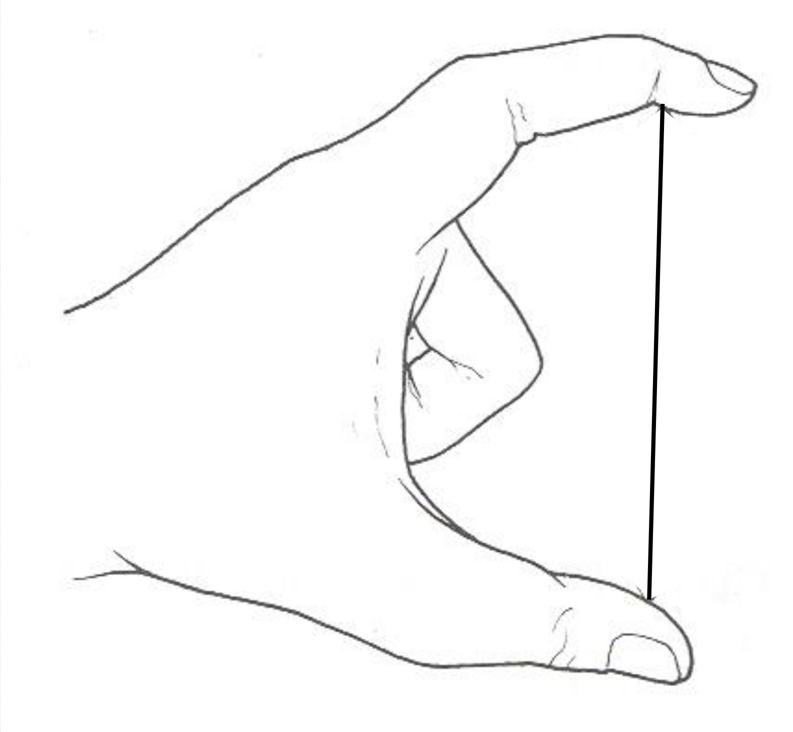
Quantum fluctuations drive "quantum phase transitions".



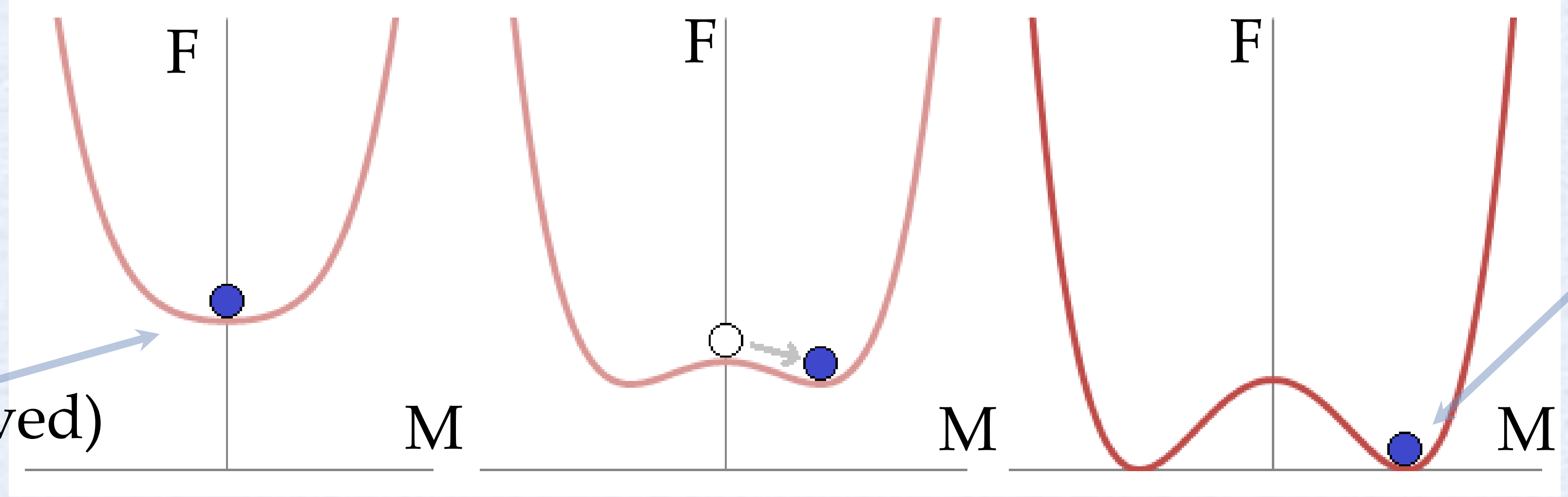
[M. Vojta, Rep. Prog. Phys. (2003)]

Quantum States of Matter: Spontaneous Breaking of Symmetries

Continuous phase transitions:



$$F[M] = aM^2 + bM^4 \text{ (Landau)}$$



no "order"
(symmetry preserved)

finite
"order parameter":
broken symmetry

How to investigate this numerically? Which quantities to compute?

expectation values:
local observables,
correlation functions, …

Unconventional States:
Topological Phases

“Topological order“: <u>beyond</u> Landau paradigm

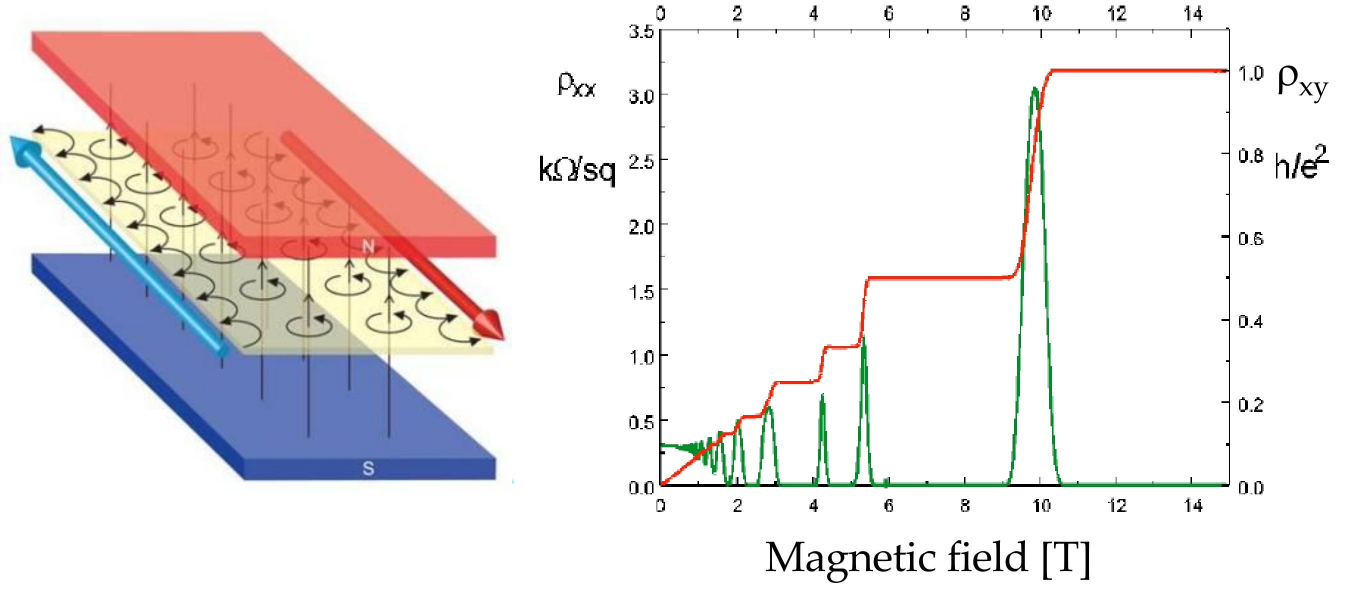
Nobel Prize 2016

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?

⇒ topological invariants, energy gaps, *entanglement* properties, „Schmidt spectrum“,…

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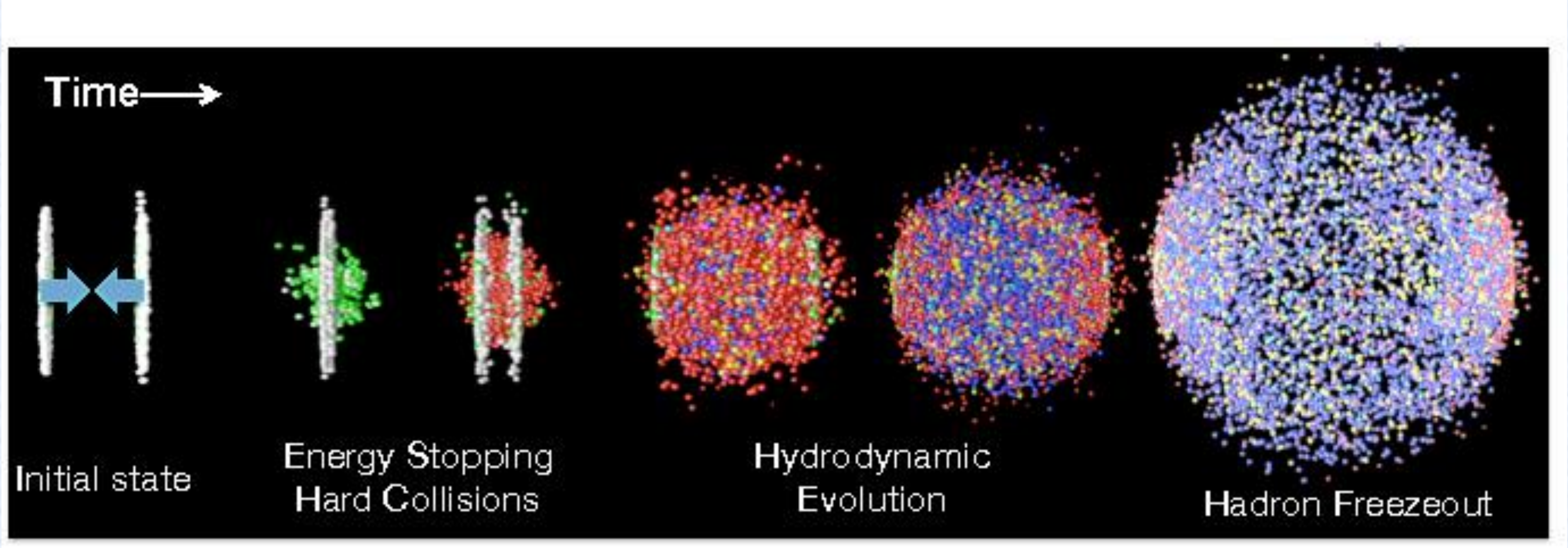
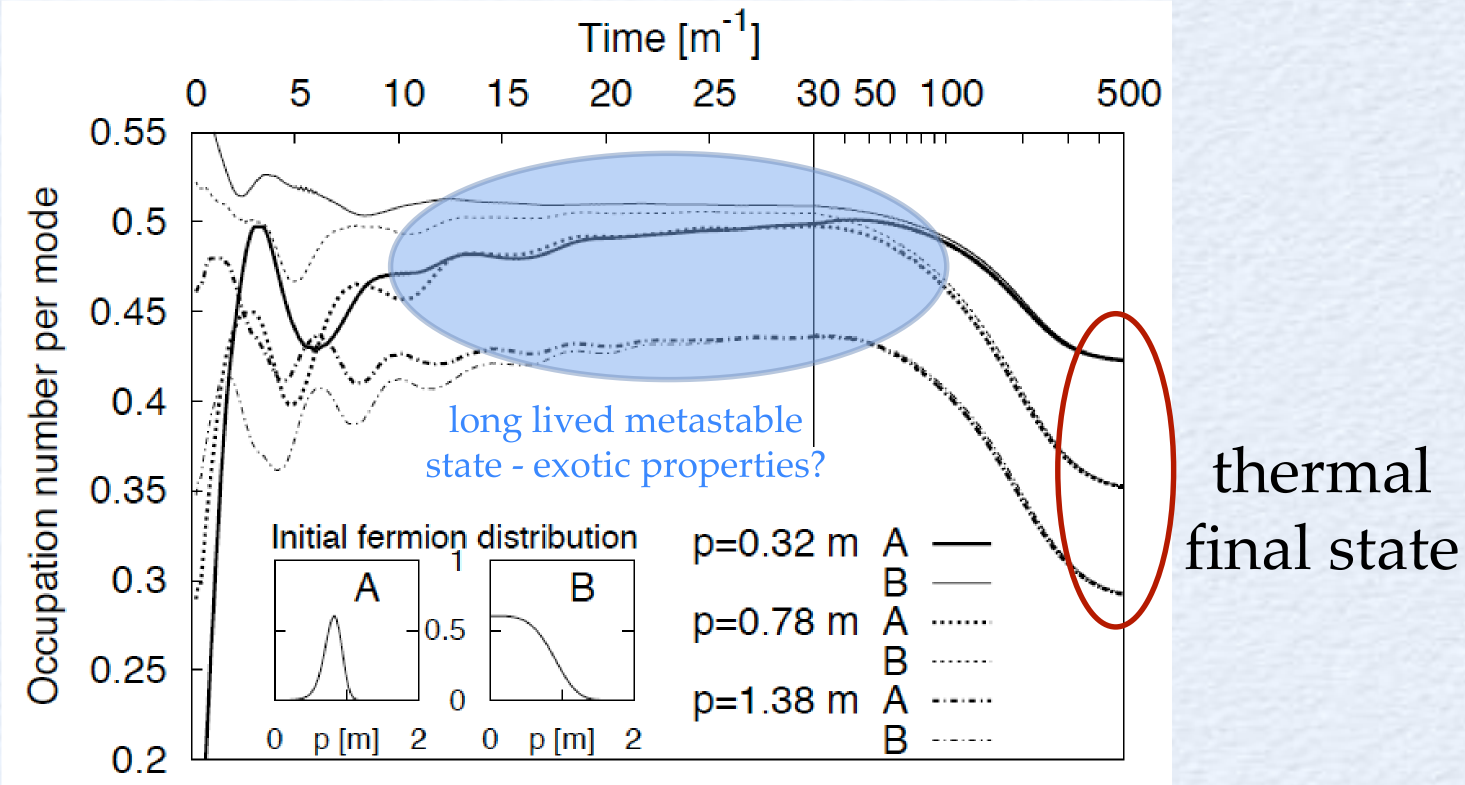
Unconventional states: Out-of-Equilibrium Dynamics

Example (high-energy physics):
heavy ion collisions



[from inspirehep.net]



[Berges *et al.*, PRL 2004]

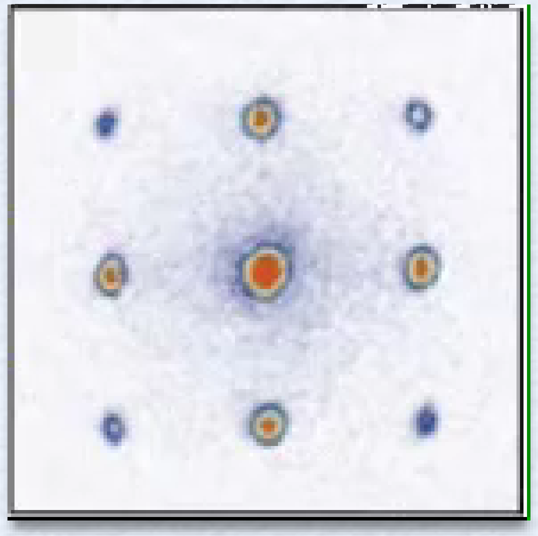
Fundamental questions:

- 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
$U_0 \rightarrow U$

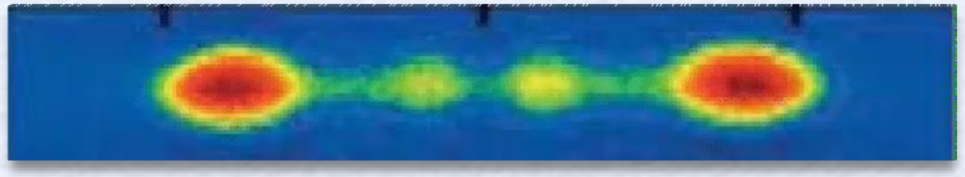


Collapse and Revival
of a Bose-Einstein-Condensate

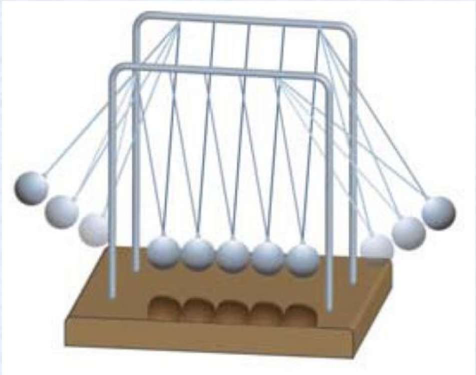
M. Greiner et al., Nature (2002)

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?

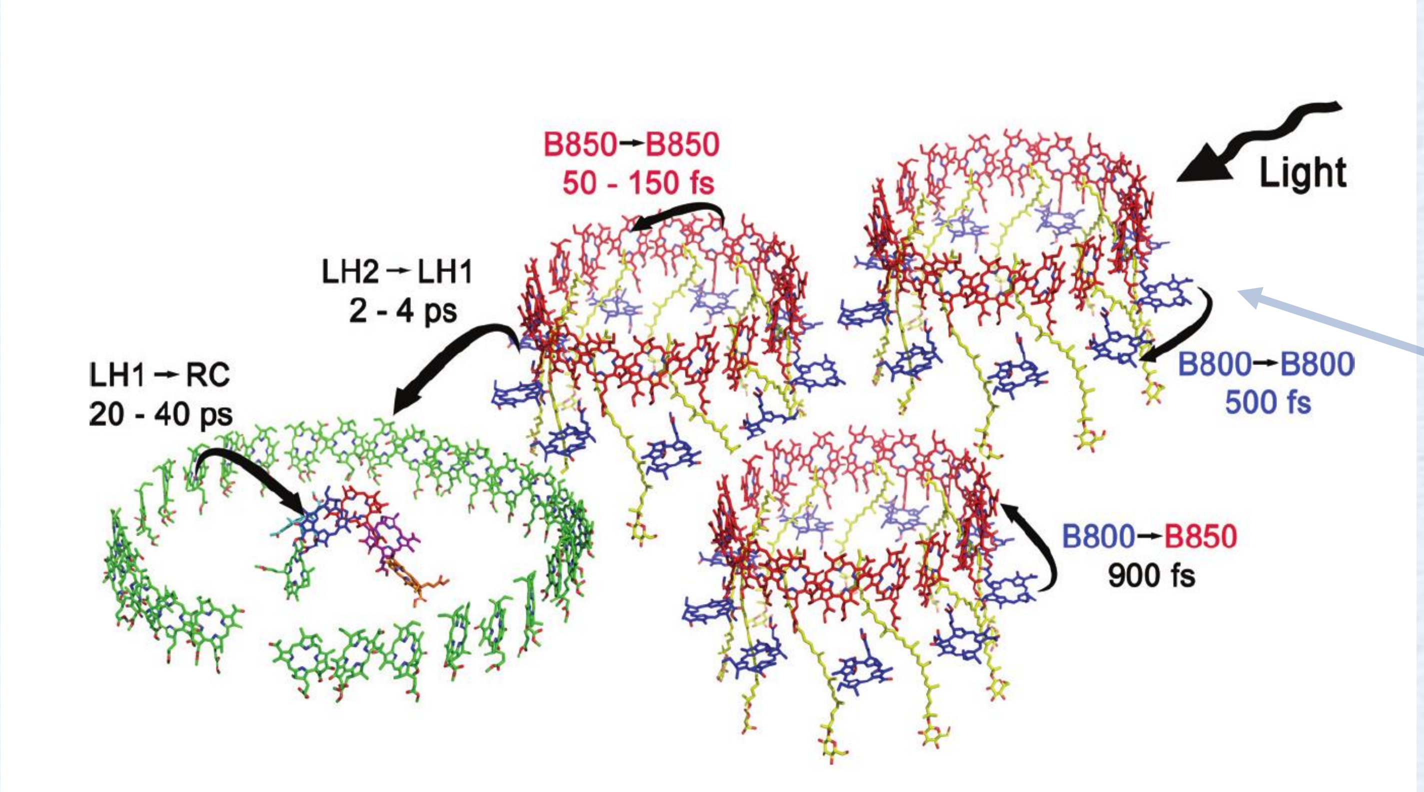
➠ accurate methods for time evolution with time-independent Hamiltonians

Many-Body Systems Out-Of-Equilibrium: Phonons

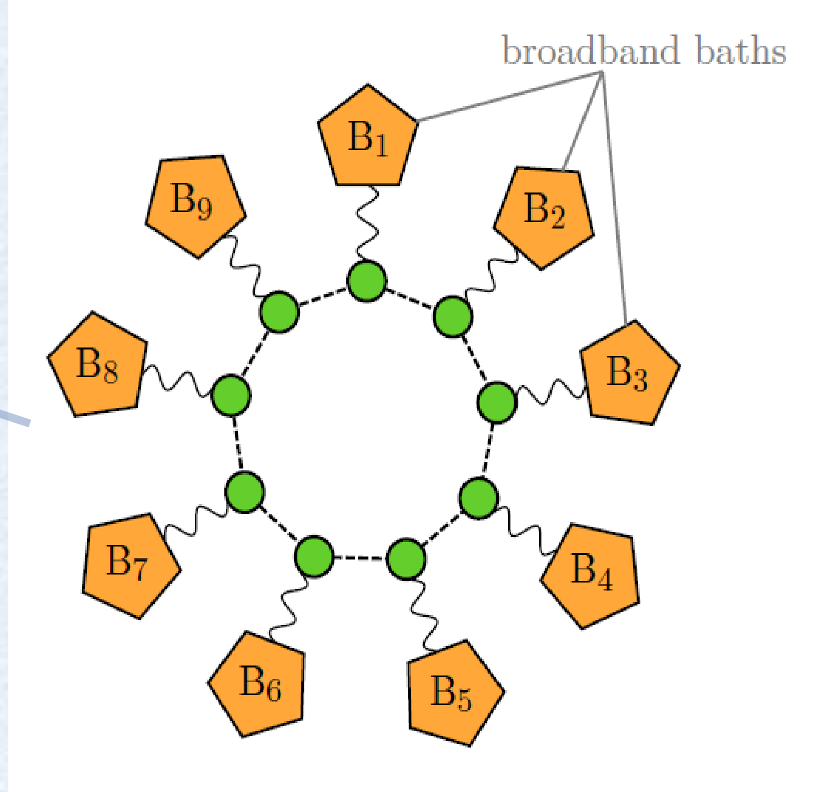
Example: light-harvesting systems

[K. Kessing, Master thesis (U. Göttingen, 2020); K. Kessing et al., in preparation]

Energy transfer in ‚antenna systems‘



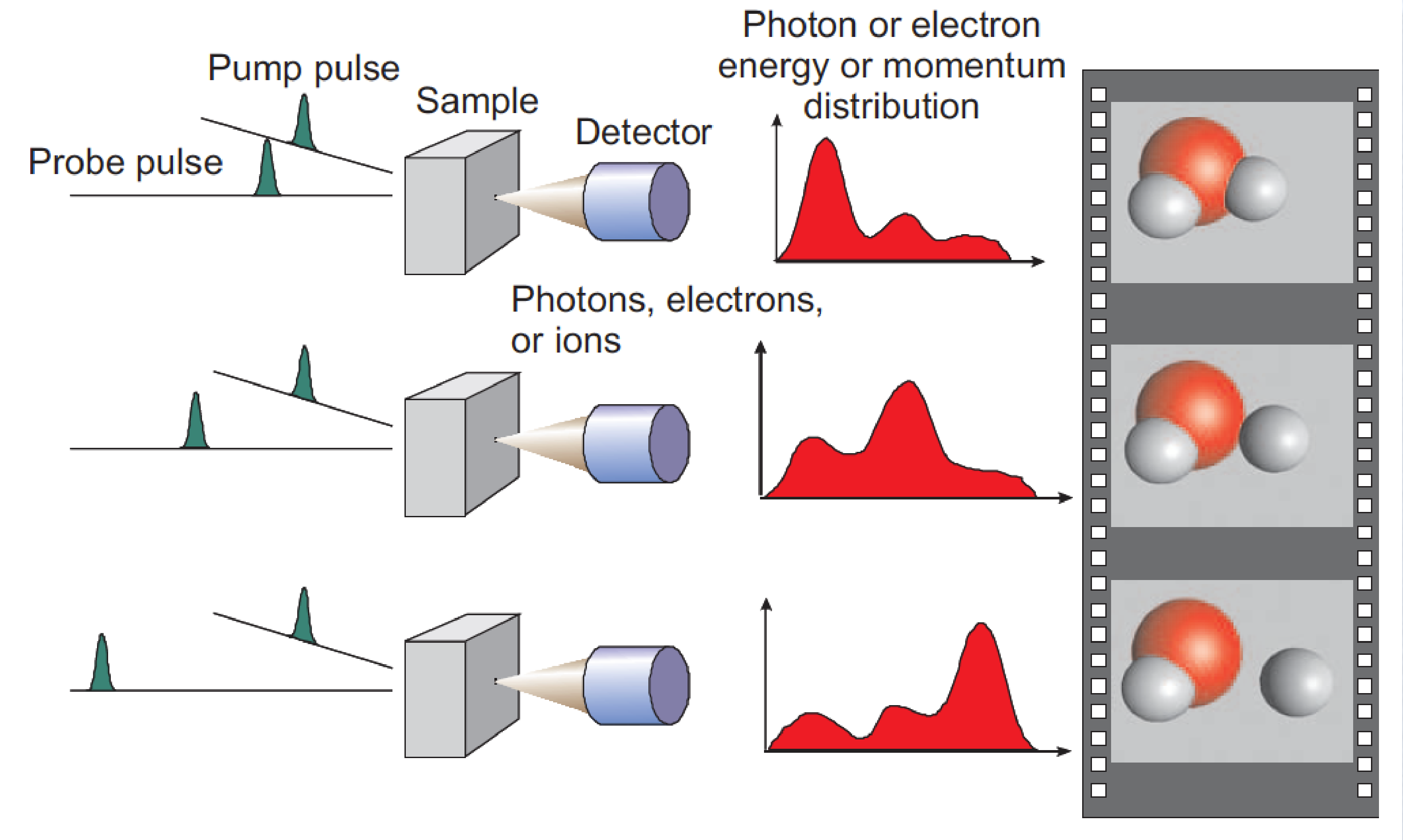
Simplified model:
ring geometry coupled to phonons



How to investigate this numerically? Which quantities to compute?

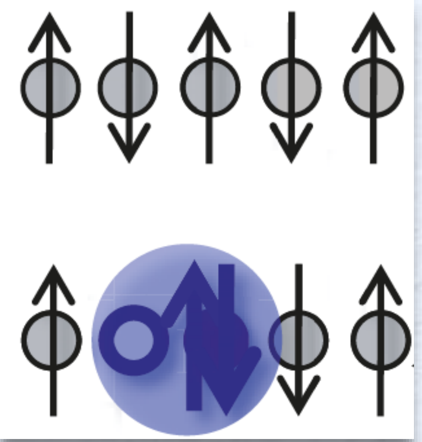
⇒ efficient approaches to treat phonons?

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



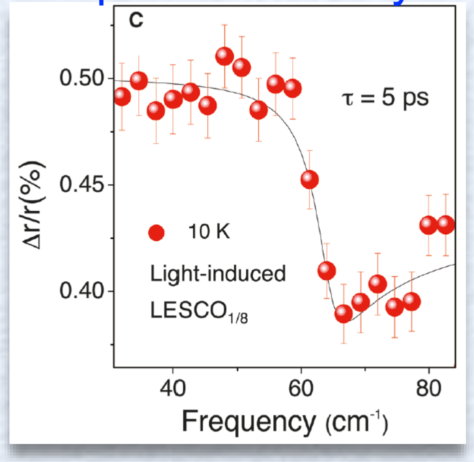
F. Krausz & M. Ivanov, RMP (2009)

Photo-excitation of Mott insulators



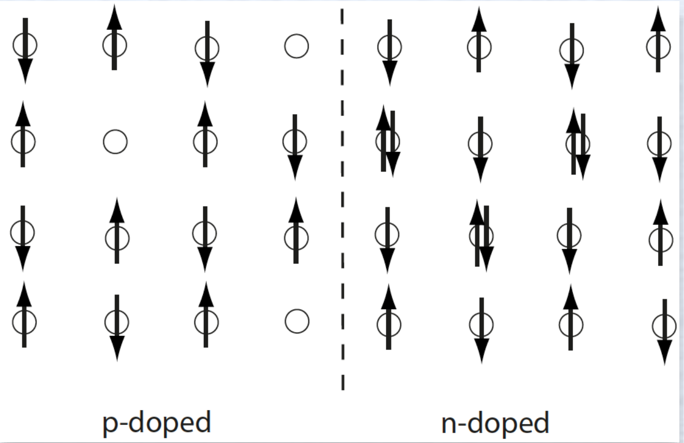
S. Wall et al., Nature Physics (2010)

"Light-induced superconductivity"



D. Fausti et al., Science (2011)

Photovoltaic effects



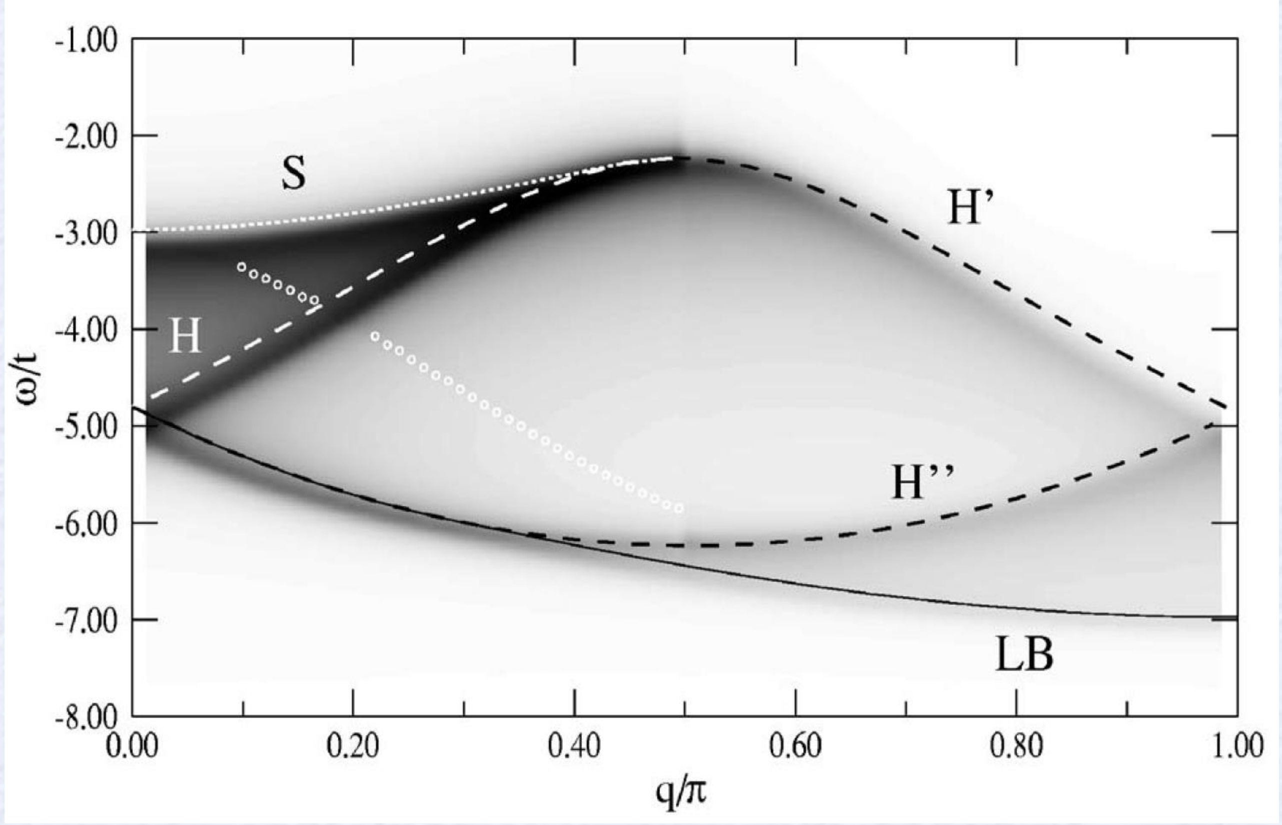
E. Manousakis PRB (2010)

How to investigate this numerically? Which quantities to compute?

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

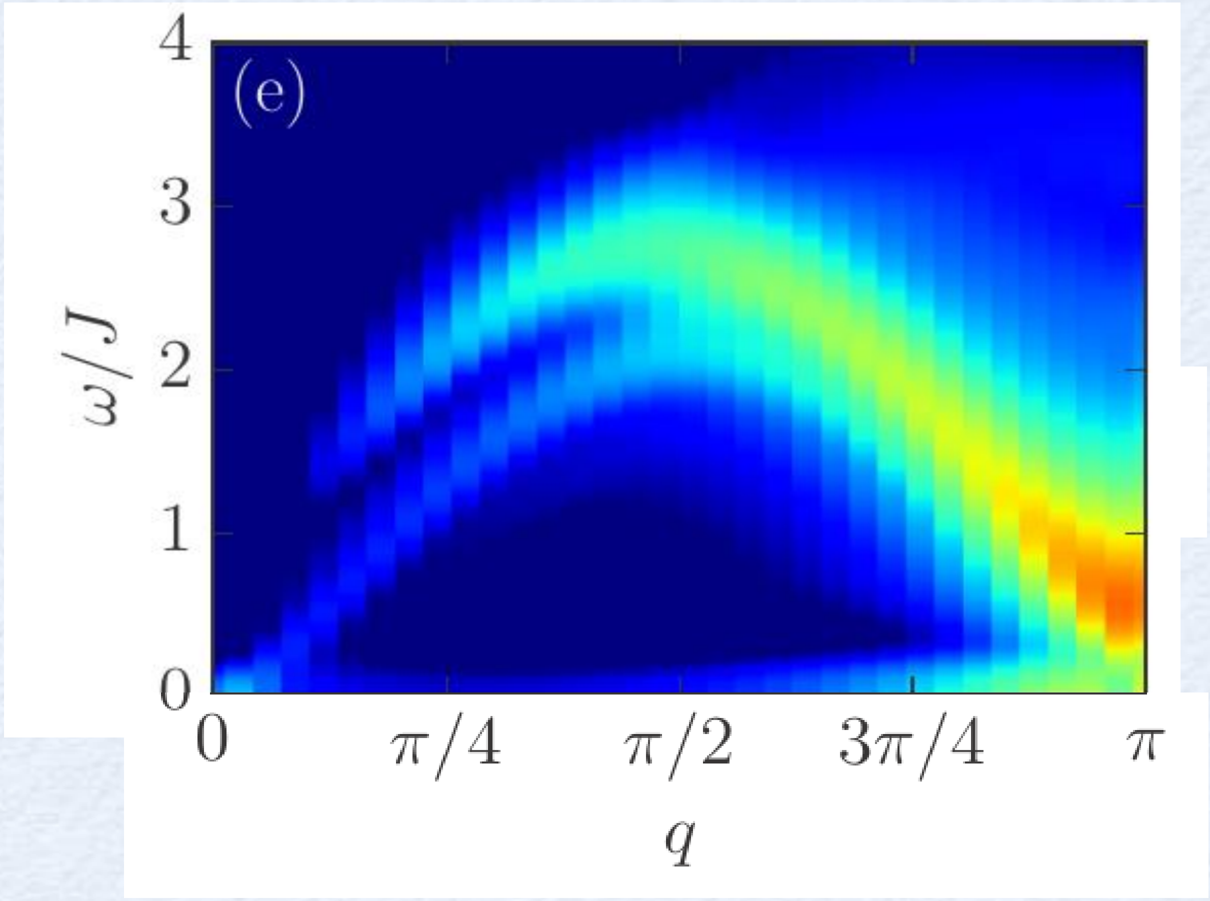
Many-Body Systems Out-Of-Equilibrium: Dynamical quantities

Ground states:
Spectral functions
(e.g., Hubbard chains)



H. Benthien & E. Jeckelmann, PRB (2007)

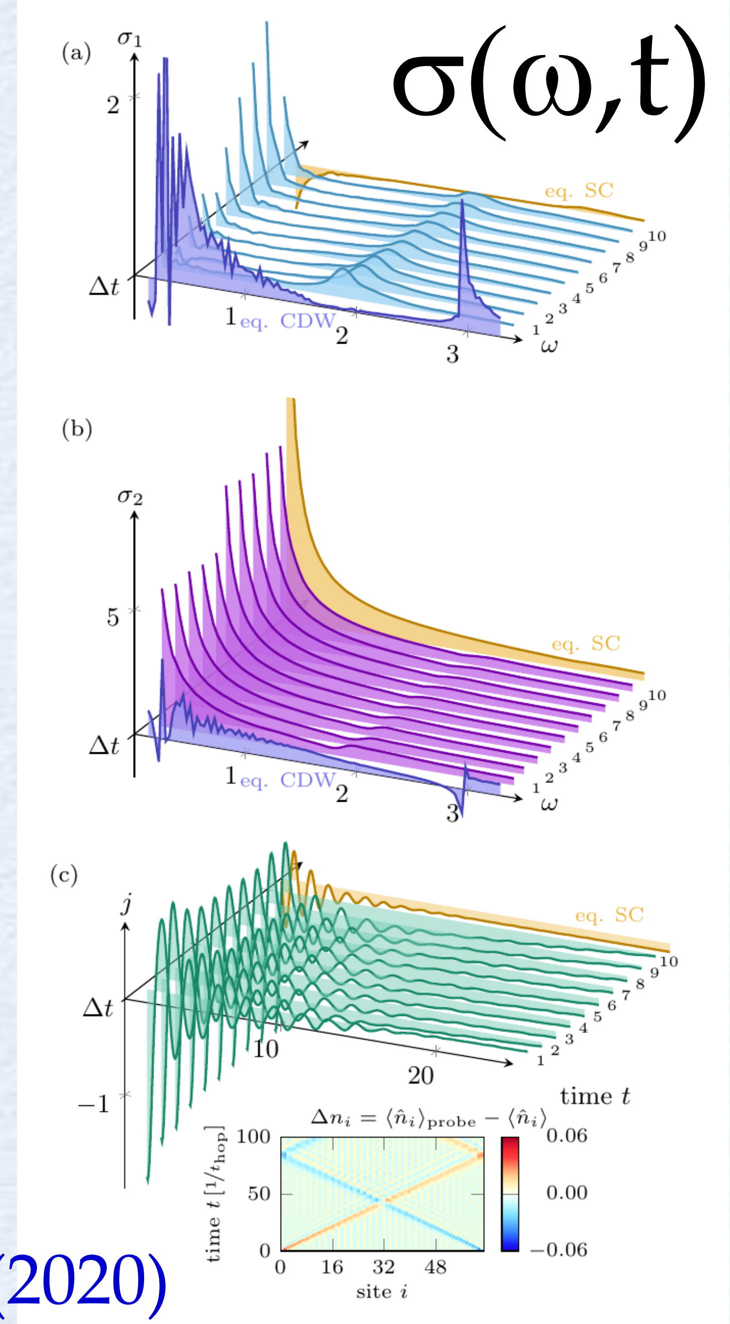
Finite temperature:
structure factors of quantum magnets
(e.g., S=1 Heisenberg chain)



J. Becker *et al.*, PRB(R) (2017)

Out-of-equilibrium:
e.g., time-dependent
optical conductivity

$\sigma(\omega,t)$

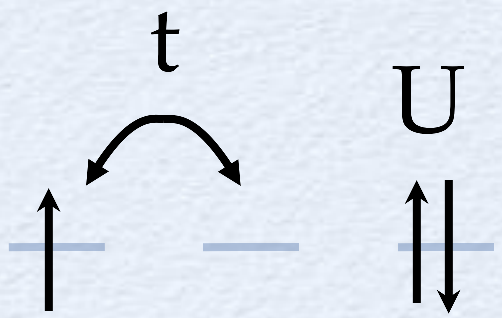


S. Paeckel *et al.*, PRB(R) (2020)

Quantum Many-Body Systems: Typical Lattice Models

Hubbard model (1D):

$$\mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} \left[c^\dagger_{i+1,\sigma} c_{i,\sigma} + h.c. \right] + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$



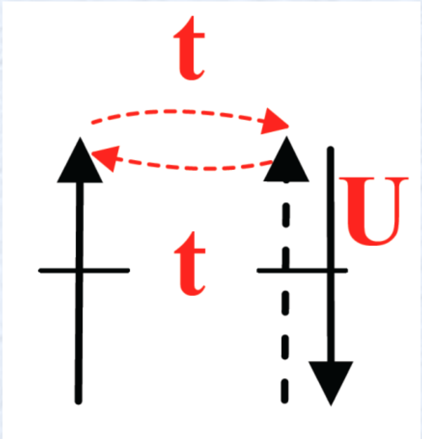
Also bosons possible:

$$H^{\mathrm{BHM}} = -J \sum_{\langle i,j \rangle} \left(b_i^\dagger b_j + h.c. \right) + \frac{U}{2} \sum_i n_i (n_i - 1)$$

Heisenberg exchange: 2nd order perturbation theory for U >> t

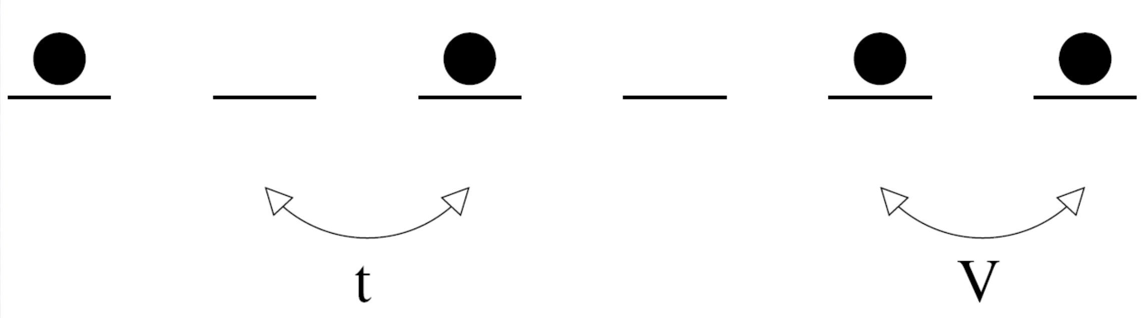
$$J\, \vec{S}_1 \cdot \vec{S}_2$$

$$J = \frac{4t^2}{U}$$



(e.g., quantum magnets)

‚Spinless Fermions'
(e.g., fully polarized extended Hubbard model):



$$\hat{H} = -t \sum_j \left(c^\dagger_{j+1} c_j + h.c. \right) + V \sum_j \hat{n}_j \hat{n}_{j+1}$$

Range of applications for MPS methods: Quantities we need to compute

We have encountered various quantities, which we need to be able to compute in order to investigate the physics of the systems of interest, for example (see hands-on session):

- Local expectation values and correlation functions, e.g. $\langle S_i^z \rangle$ and $\langle S_i^z S_j^z \rangle$
- Energy gaps: ground state energies with different quantum numbers, e.g., spin gap,

$$\Delta_S = E_0(S^z_{\text{total}} = 1, L) - E_0(S^z_{\text{total}} = 0, L)$$

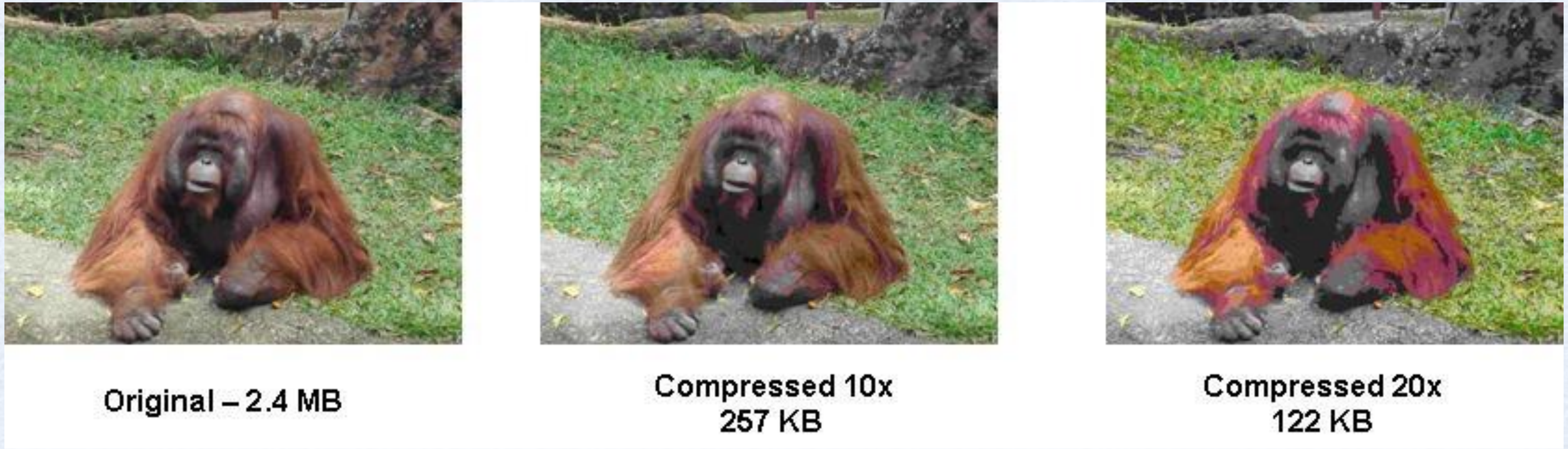
  Thermodynamic limit? Large system sizes!

- Entanglement properties, e.g., von Neumann or Entanglement Entropy $S = -\mathrm{Tr}\varrho \log \varrho$
- Dynamical spectral functions, e.g.,

$$S^{zz}(q,\omega) = \frac{1}{L}\sum_j e^{-iq(j-L/2)} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle S_j^z(t) S_{L/2}(0) \rangle$$

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.

DMRG Algorithms:
Key Aspects

S.R. White, PRL (1992); U. Schollwöck, RMP (2005)/Ann. Phys. (2011); **R.M. Noack & S.R.M., AIP (2005)**

Schmidt decomposition:
(see black board)

$$|\psi\rangle = \sum_{j=1}^{\dim\mathcal{H}} w_j\, |\alpha\rangle_j\, |\beta\rangle_j \approx \sum_{j=1}^{m} w_j\, |\alpha\rangle_j\, |\beta\rangle_j$$

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

Approximation: $m \ll \dim\mathcal{H}$
(e.g., 1000 sites:
$\dim\mathcal{H} = 2^{1000} > (1 \text{ googol})^3$.
Typical choice: $m = 800$)

$|\alpha\rangle_j, |\beta\rangle_j$: eigenstates of the reduced density matrix of A or B

- *very powerful in 1D*
- nonequilibrium, finite-T, linear-response dynamics

A. Daley *et al.*, J.Stat. (2004);
S.R. White & A.E. Feiguin, PRL (2004);
S.R.M. *et al.*, AIP (2005);
R.M. Noack, **S.R.M.** *et al.*, Springer Lect. Notes (2008);
A.C. Tiegel, **S.R.M.**, *et al.*, PRB(R) (2014)
Recent Review: S. Paeckel *et al.*, Ann. Of Phys. *(2019)*

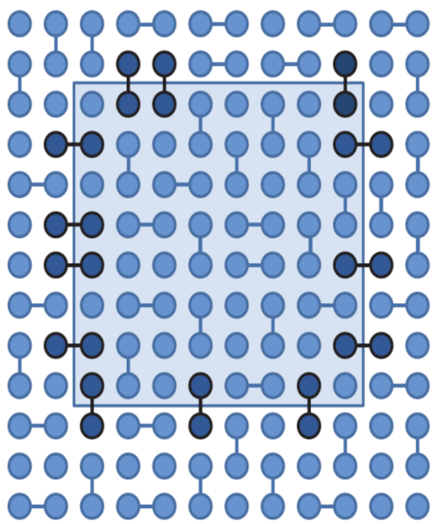
Key: entanglement entropy $\quad S = -\sum_j w_j^2 \log w_j^2$

➥ the larger the entanglement in the system, the larger *m*

Problem in 2D:
"area law of entanglement" - *m* grows exponentially with system size

➥ Frontier of today's efforts.

2D:



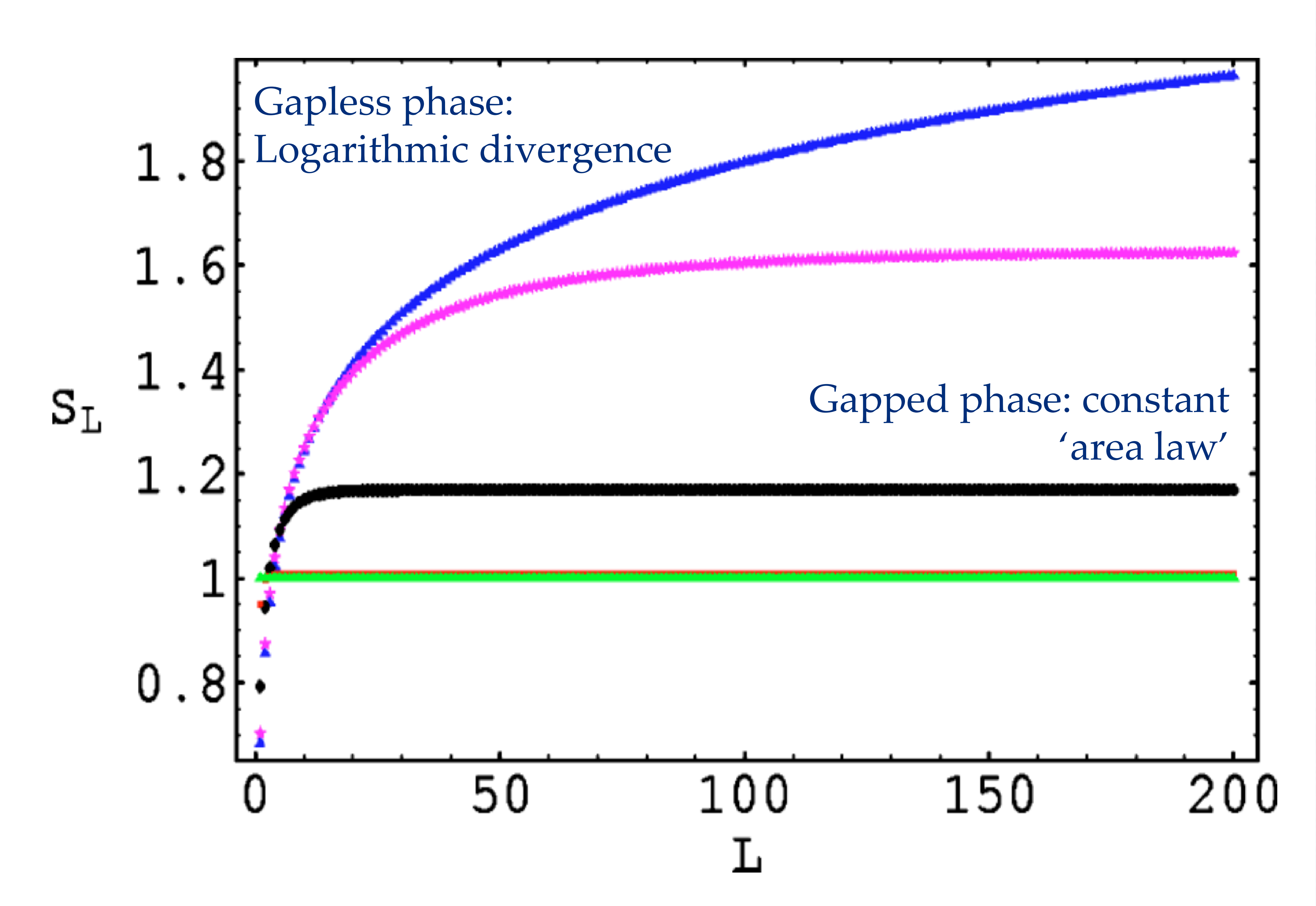
[See, e.g., E.M. Stoudenmire & S.R. White, Ann. Rev. Cond. Mat. Phys. (2012).]

DMRG:

Entanglement Area Law

[U. Schollwöck, Rev. Mod. Phys. (2005)]

Entanglement Entropy in 1D (Ising-model in transv. field)

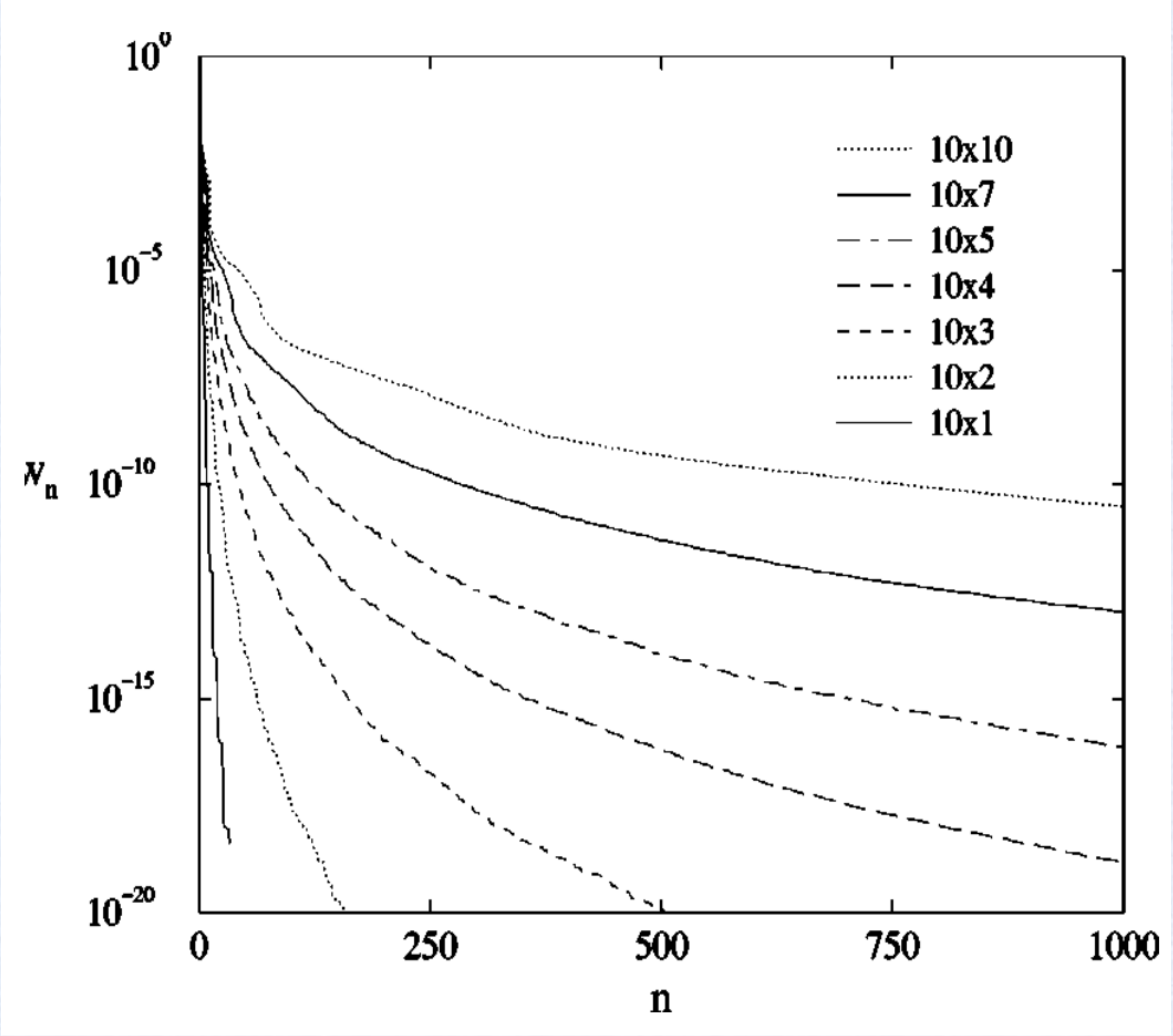


DMRG:
Truncation efficiency in 1D and in 2D

[U. Schollwöck, Rev. Mod. Phys. (2005)]

From 1D to 2D: Schmidt values

$$|\psi\rangle = \sum_{j=1}^{\dim\mathcal{H}} w_j \, |\alpha\rangle_j \, |\beta\rangle_j \approx \sum_{j=1}^{m} w_j \, |\alpha\rangle_j \, |\beta\rangle_j$$



Need to keep much larger number of states to reach same accuracy!

DMRG:

Too much entanglement…

…is just annoying.

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):

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

➟ 2·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?

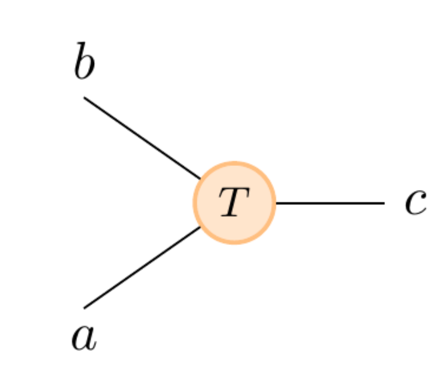
Consider the following two aspects:

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!

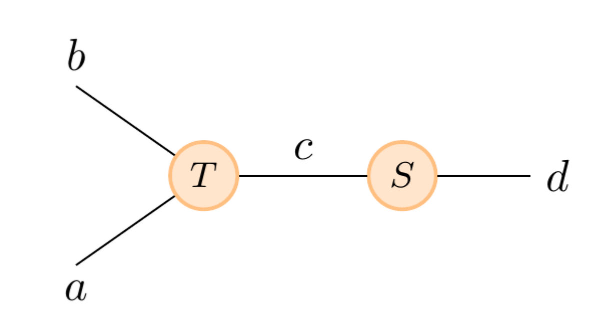
Good to know & very useful: Graphical Representation

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

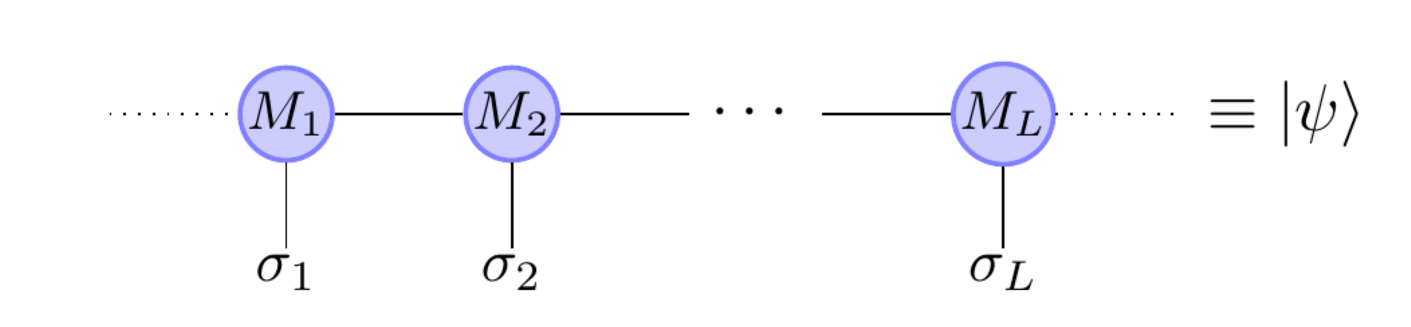


[This is also called *Penrose graphical notation of tensors*, R. Penrose (1971)]

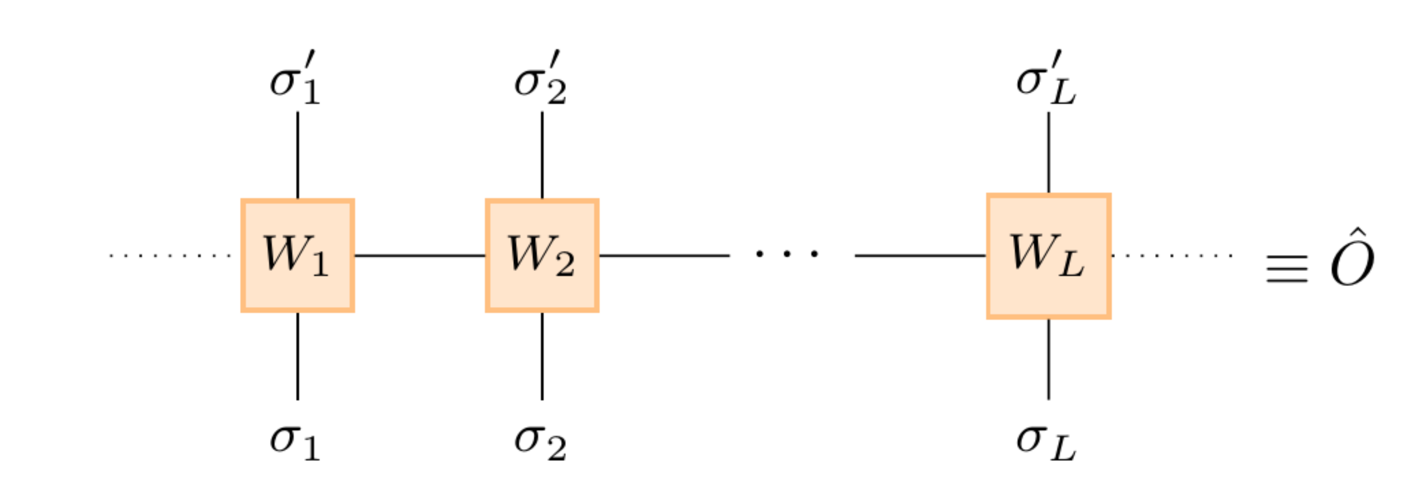
Contraction of two indices
(multiplication of two matrices)



Matrix Product State:



Matrix Product Operator:

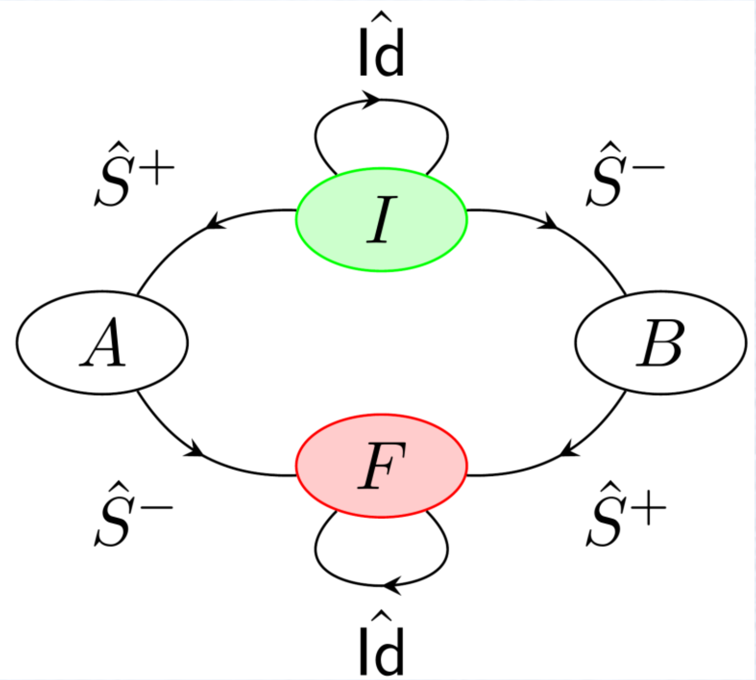


Useful representation of MPO-matrices: Finite states machines

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

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

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



[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]

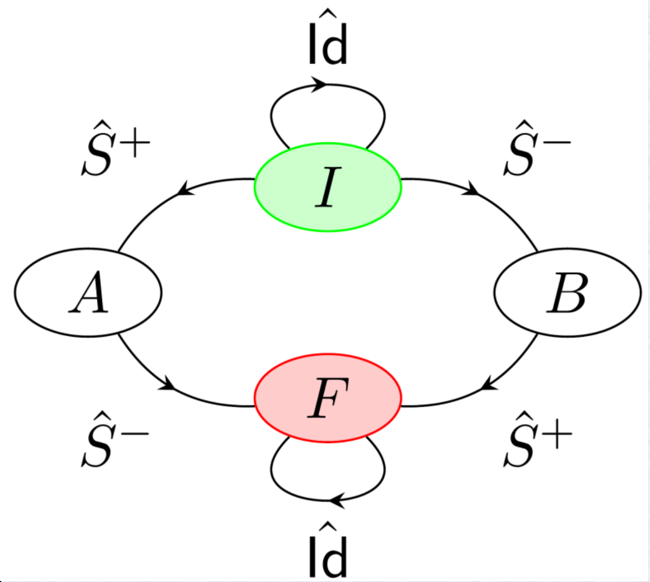
Properties & Advantages:

- 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

Useful representation of MPO-matrices: Finite states machines

[SymMPS package, https://www.symmps.eu]

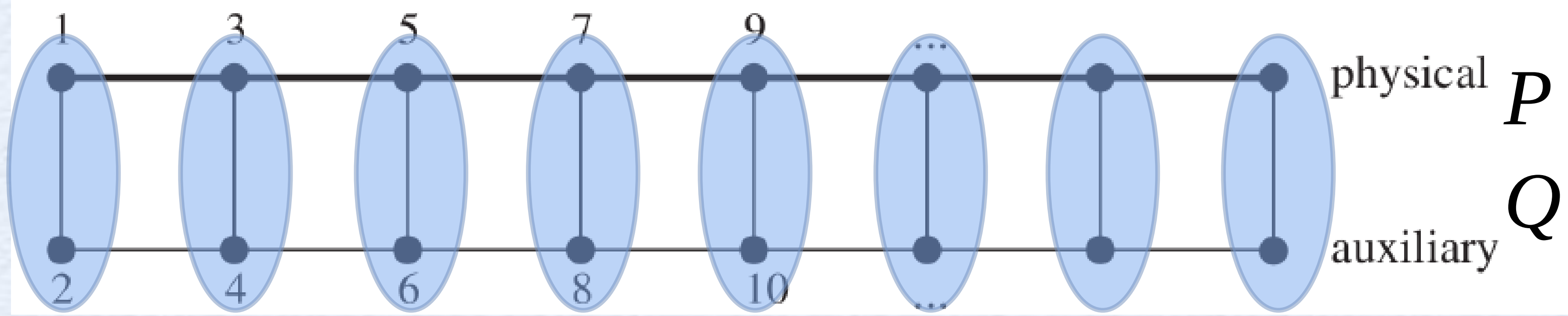
$$\hat{H}_{XX} = \sum_i \hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+$$




```
subsection xx
        set parameters          =       J
        set description         =       "XX-Model with OBC: \begin{align}\sum_{j=0}^{L-1} \
left[ J_j \left( \hat S^+_j \hat S^-_{j+1} + \hat S^-_j \hat S^+_{j+1} \right) \end{align}"
        set transitions         =       I:Id:I; F:Id:F; \
                                        \
                                        I:J*Splus:A; A:Sminus:F; \
                                        I:J*Sminus:B; B:Splus:F;
        set print_ignore        =       Id
        set weight_functions    =       J: { 0.5 * J}
end
```

Finite temperature methods: purification & matrix product states

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



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

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

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

Purification:
“Thermofields” in Liouville Space

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

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

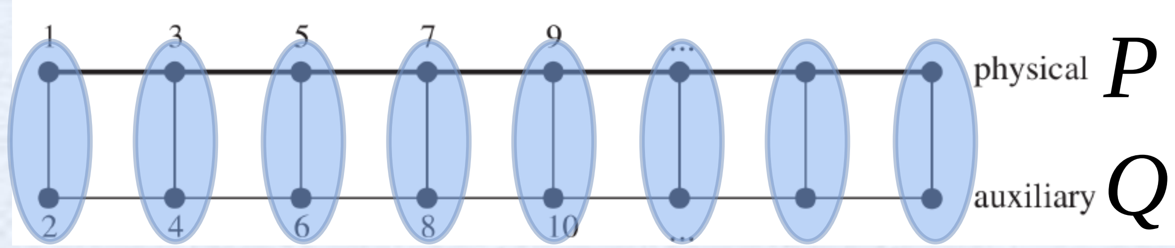
von Neumann equation

Liouville equation

Finite temperature methods: purification & matrix product states

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

Purification:



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

$$\left[\otimes_{j=1}^{L} |\mathrm{rung}-\mathrm{singlet}\rangle_j\right]$$

1. Schmidt decomposition „backwards“:

$$\hat{\rho}_P = \sum_{a=1}^{r} s_a^2 |a\rangle_P \langle a|_P \to |\psi\rangle = \sum_{a=1}^{r} s_a |a\rangle_P |a\rangle_Q \qquad \hat{\rho}_P = \mathrm{Tr}_Q |\psi\rangle\langle\psi|$$

2. Rewrite:

$$\hat{\rho}_\beta = Z(\beta)^{-1} \mathrm{e}^{-\beta\widehat{H}} = Z(\beta)^{-1} \mathrm{e}^{-\beta\widehat{H}/2} \cdot \widehat{I} \cdot \mathrm{e}^{-\beta\widehat{H}/2}$$

3. Choose/construct $|\psi_0>$ so that $Z(0)\,\rho_0 = \hat{I}$

4. Rewrite:

$$\hat{\rho}_\beta = (Z(0)/Z(\beta))\mathrm{e}^{-\beta\widehat{H}/2} \cdot \mathrm{Tr}_Q |\psi_0\rangle\langle\psi_0| \cdot \mathrm{e}^{-\beta\widehat{H}/2} = (Z(0)/Z(\beta))\mathrm{Tr}_Q \mathrm{e}^{-\beta\widehat{H}/2} |\psi_0\rangle\langle\psi_0| \mathrm{e}^{-\beta\widehat{H}/2}$$

→ Need to compute imaginary time evolution $|\psi_\beta\rangle = \mathrm{e}^{-\beta\widehat{H}/2}|\psi_0\rangle$

5. Compute expectation values:

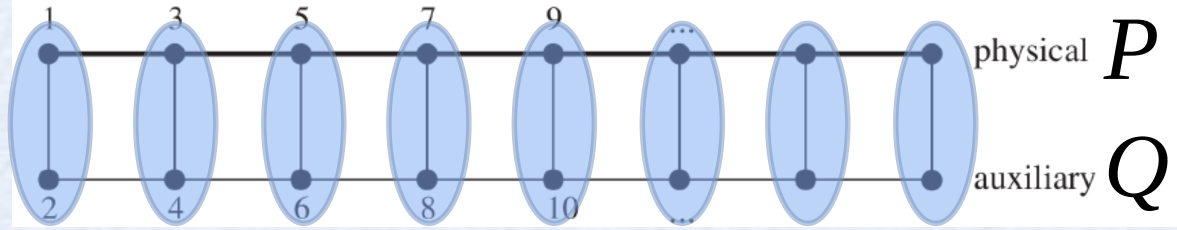
$$\langle\widehat{O}\rangle_\beta = \mathrm{Tr}_P \widehat{O}\hat{\rho}_\beta = (Z(0)/Z(\beta))\mathrm{Tr}_P \widehat{O} \mathrm{Tr}_Q |\psi_\beta\rangle\langle\psi_\beta| = (Z(0)/Z(\beta))\langle\psi_\beta|\widehat{O}|\psi_\beta\rangle$$

6. Partition function via:

$$1 = \langle\widehat{I}\rangle_\beta = \mathrm{Tr}_P \hat{\rho}_\beta = (Z(0)/Z(\beta))\mathrm{Tr}_P \mathrm{Tr}_Q |\psi_\beta\rangle\langle\psi_\beta| = (Z(0)/Z(\beta))\langle\psi_\beta|\psi_\beta\rangle$$

Finite temperature methods: purification & matrix product states

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



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

Note: **Partition function** can be computed as

$$Z(\beta)/Z(0) = \langle \psi_\beta | \psi_\beta \rangle$$

With $Z(0) = d^L$ (d: dimension of the Hilbert space on a site, L: number of sites in P)

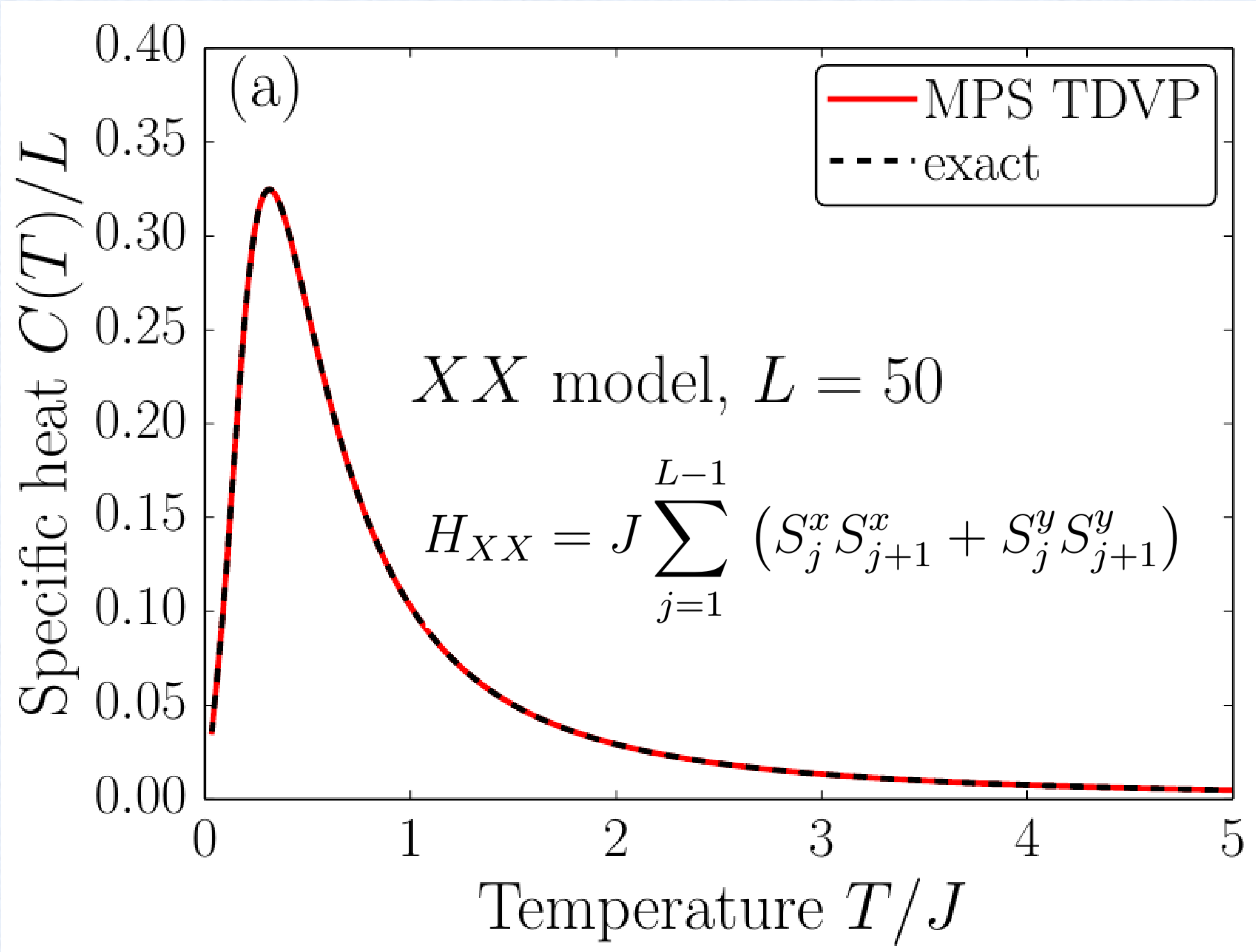
This allows one to compute thermodynamic quantities via expectation values, thermodynamic relations, and the free energy,

$$F(\beta) = -\beta^{-1} \ln Z(\beta)$$

Finite temperature methods: purification & matrix product states

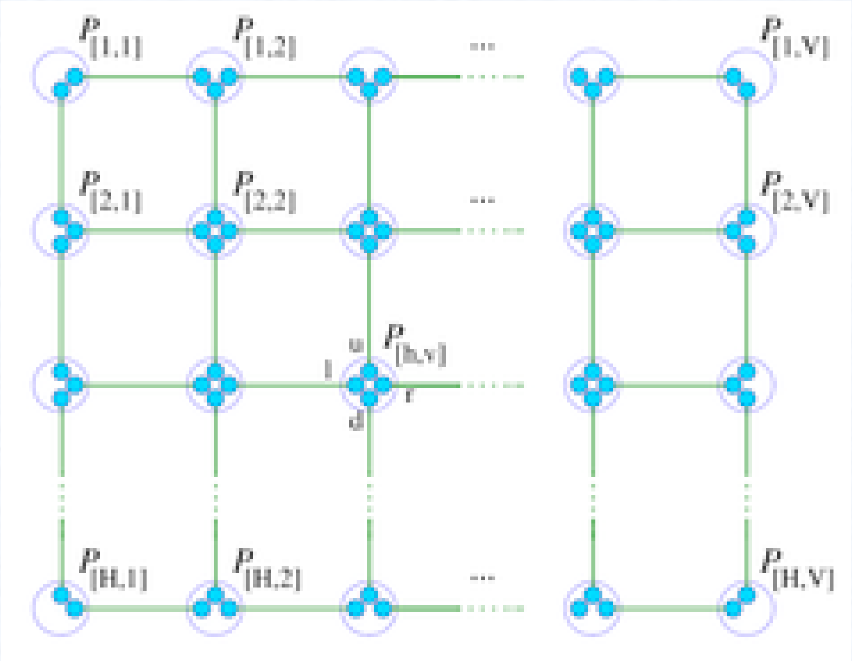
Example:

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



Outlook 2D:
PEPS, MERA & Tensor Networks

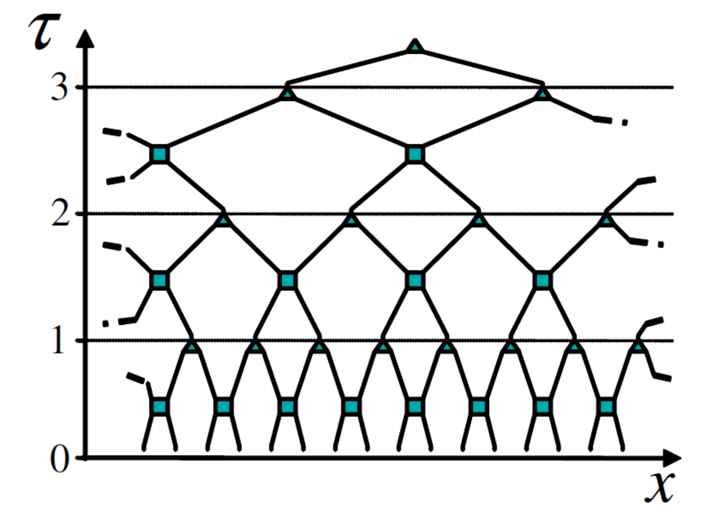
Projected Entangled Pair States (PEPS): F. Verstraete & I. Cirac, arXiv (2004)



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

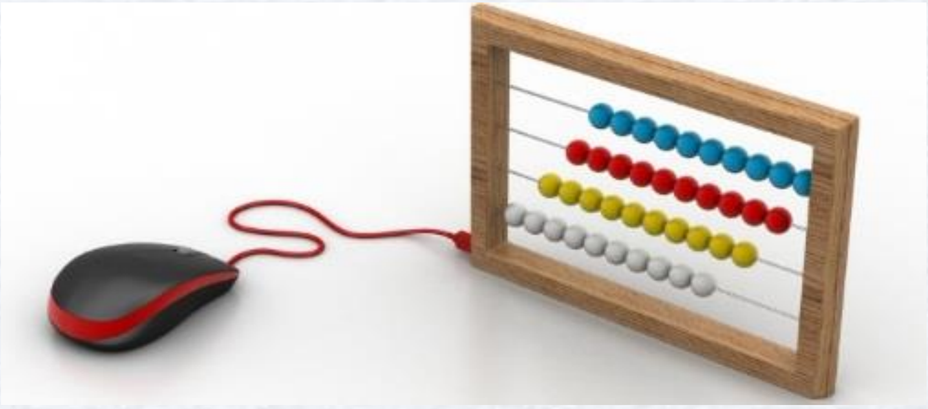
with $[A_i]^k_{l,r,u,d}$ *tensors (e.g., square lattice: rank-4)*

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



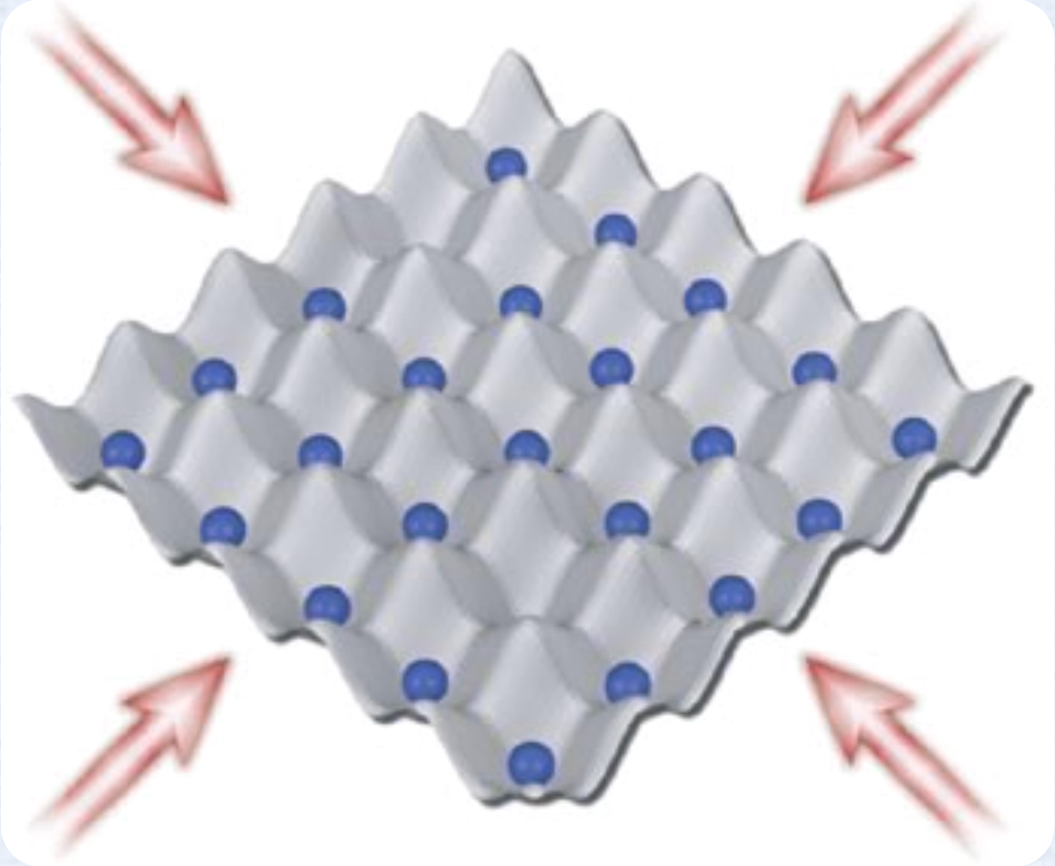
control of entanglement via unitary transforms:
'disentanglers' + block renormalization

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



Many-Body Systems Out-Of-Equilibrium: Ultracold Gases & Optical Lattices

[I. Bloch et al., Rev. Mod. Phys. **80**, 885 (2008)]



Standing waves of laser light: periodic structures

Mechanism: Stark-Effect

➠ Induced dipolemoment in neutral atoms leads to a trapping force in the periodic potential: “Crystals of Light”

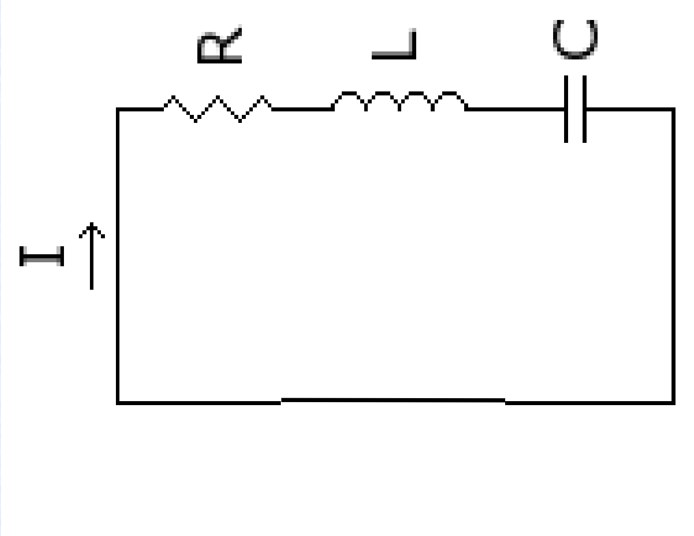
Quantum Simulators: Correlated Systems

[I. Bloch et al., Nat. Phys. **8**, 267 (2012)]

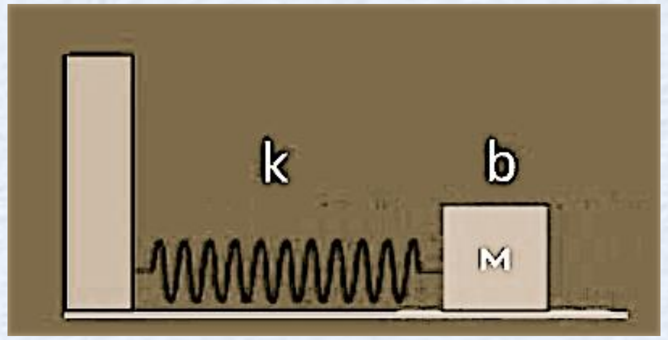
Idea: Use a well controlled quantum system to describe another, more difficult one (R.P. Feynman 1982, Y.I. Manin 1980)

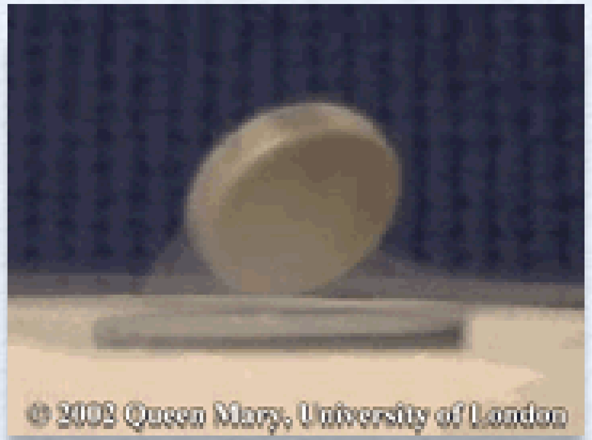
➥ Quantum-Many-Body-*Models* via ultracold gases on optical lattices

Similarity: compare electrical and mechanical networks



⟷





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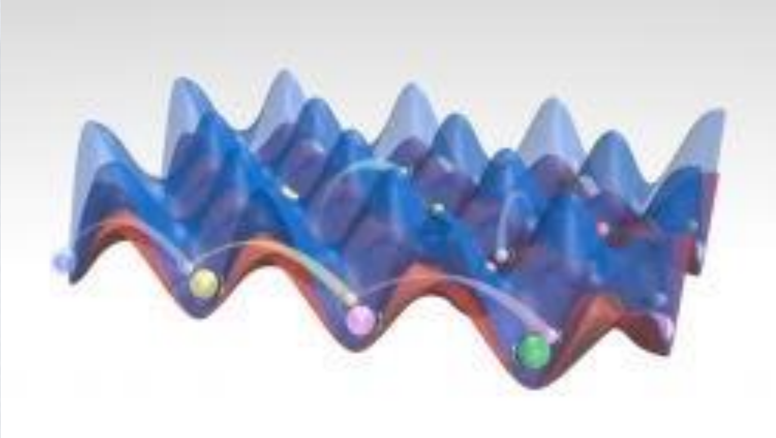
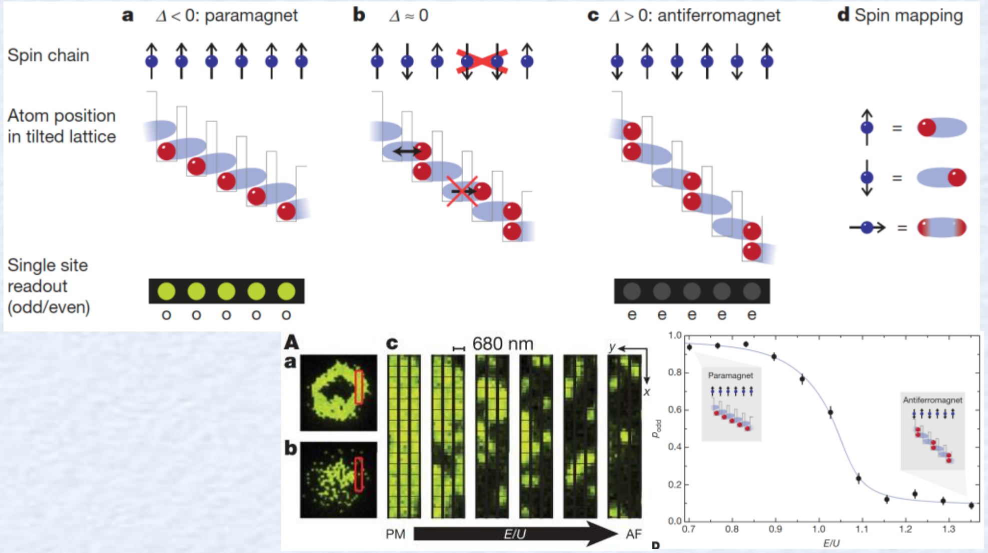


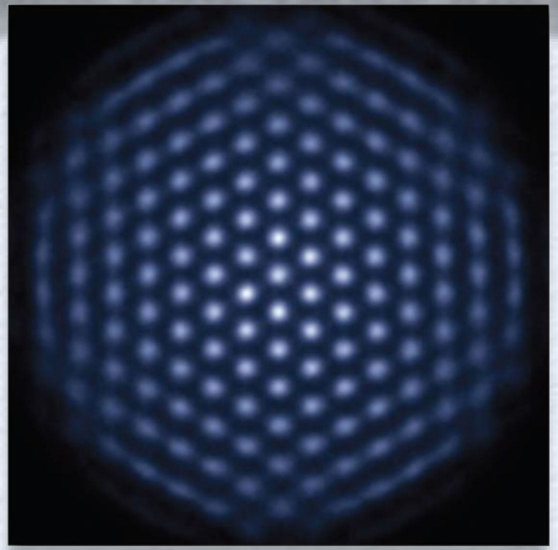
Salvatore R. Manmana

Quantum Simulators:
some developments

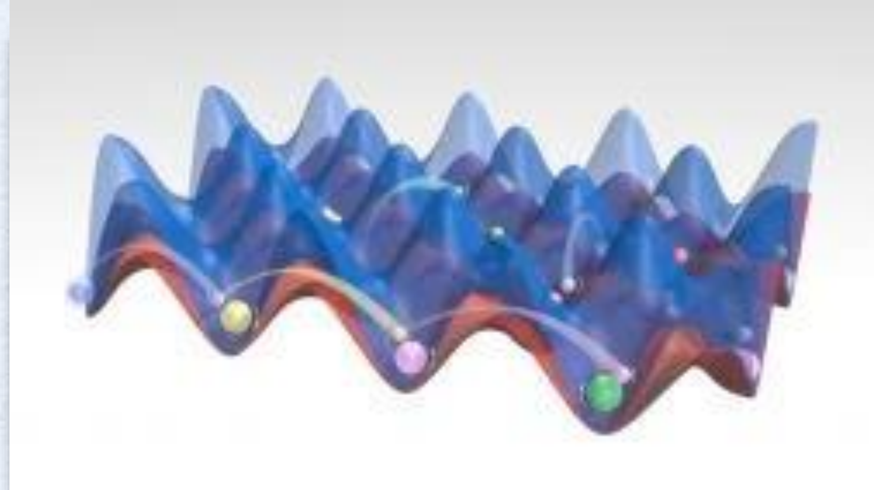
Tilted Mott insulators:
Quantum Ising models



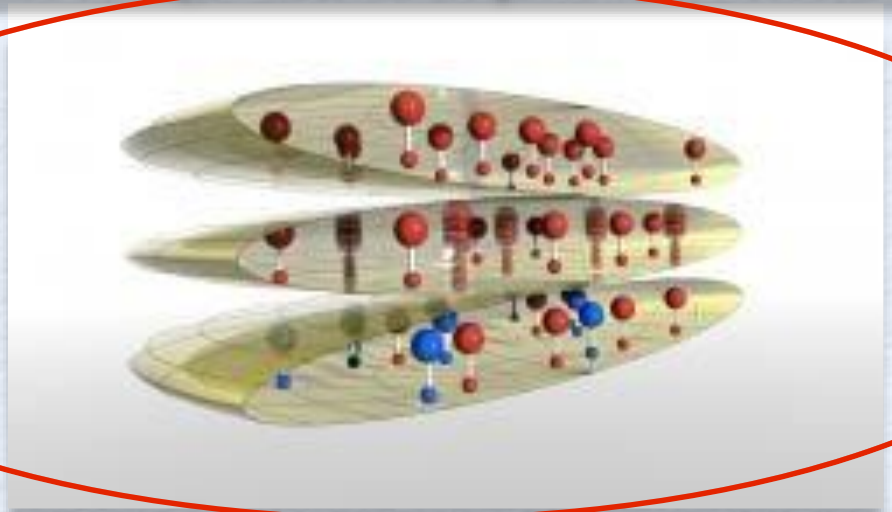
Be[9+] ions in a trap:
frustrated Ising systems with
tunable long-range interactions



Ultracold atoms (alkaline, alkaline earths) :
SU(2) and SU(N) Hubbard models



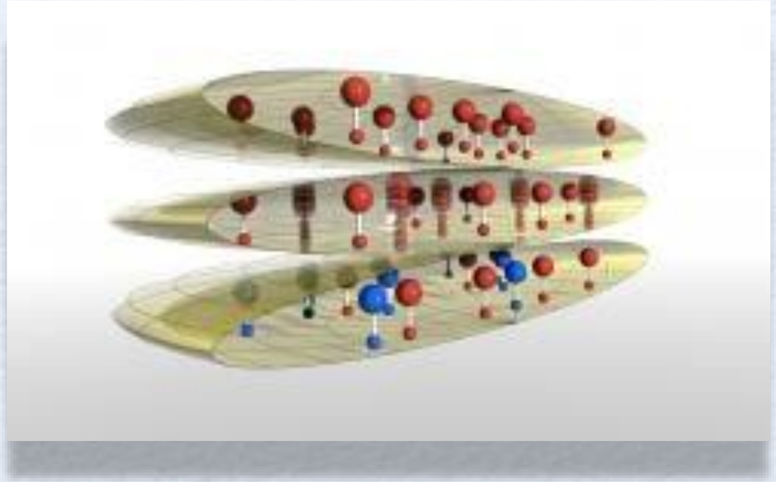
Ultracold polar molecules (KRb, LiCs,...):
spin- and t-J-models
(quantum magnetism, superconductivity,...)



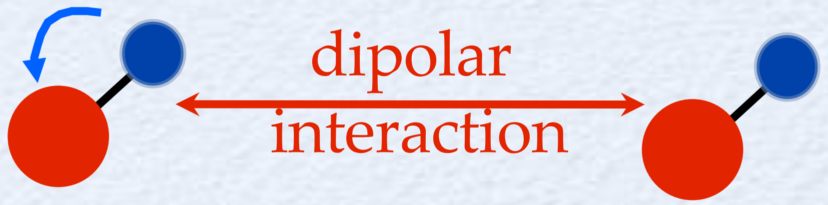
Salvatore R. Manmana

Ultracold polar molecules
dipolar t-J-V-W Model

[A.V. Gorshkov, S.R. Manmana et al., PRL & PRA (2011)]

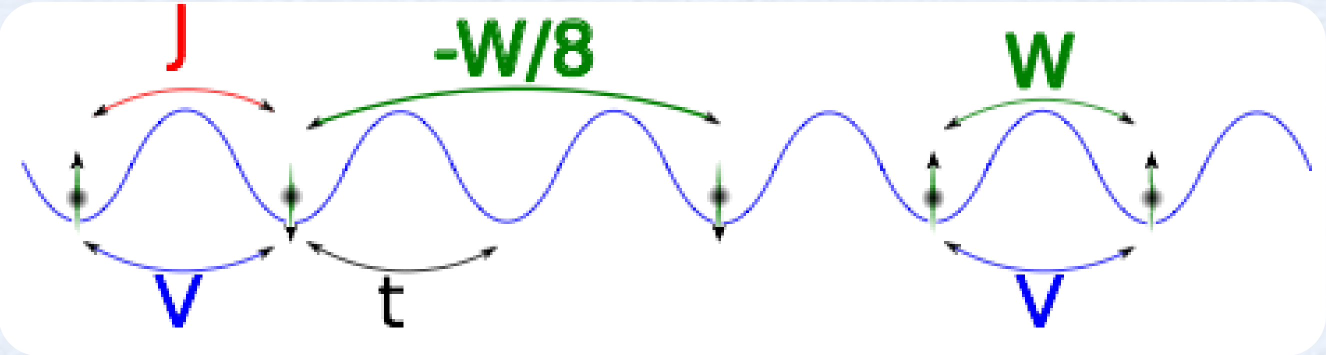


polar Molecules (e.g. KRb) in optical lattices:
2 Rotational states ⇔ two Spinstates



Effective Model:

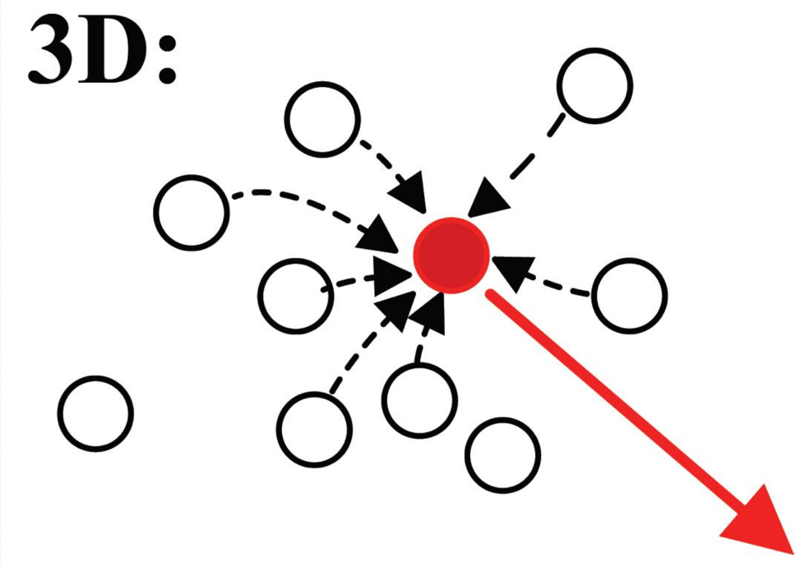
$$\mathcal{H} = -t\sum_{j,\sigma}\left[c^{\dagger}_{j,\sigma}c_{j+1,\sigma} + h.c.\right] + \sum_{i,j}\frac{1}{|i-j|^3}\left[\frac{J_\perp}{2}\left(S^+_i S^-_j + S^-_i S^+_j\right) + J_z S^z_i S^z_j + V n_i n_j + W\left(n_i S^z_j + S^z_i n_j\right)\right]$$



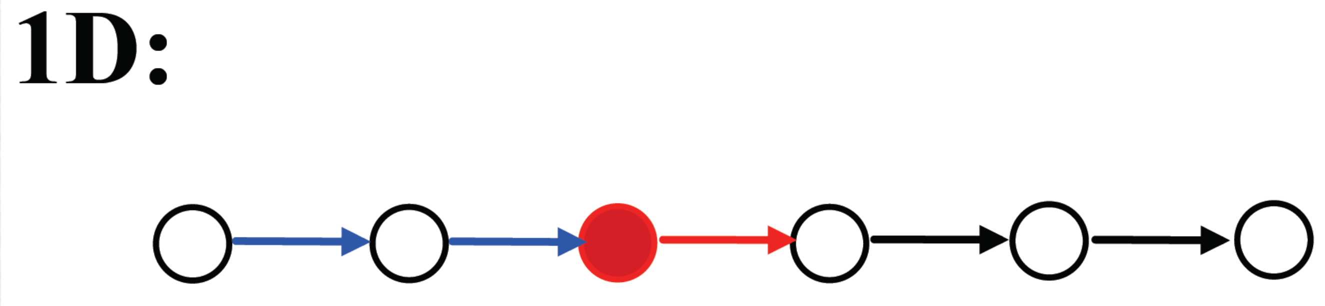
t: nearest-neighbor hopping
V: Coulomb-repulsion (long-range)
W: density-spin-interaction (long-ranged)
J: Heisenberg coupling (anisotropic, long-ranged)

Simplest case: weak E-fields
➠ $J_z = V = W = 0$, 1D for DMRG
➥ dipolar t-$J_\perp$-chain

One-Dimensional Systems: Luttinger Liquids

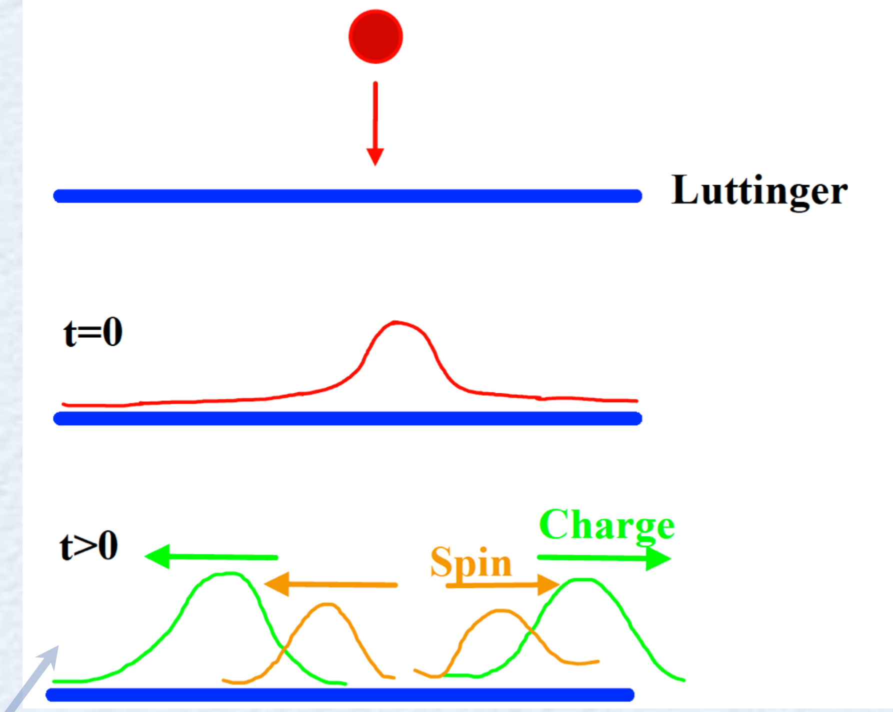


Fermi liquid:
quasi-free quasiparticles

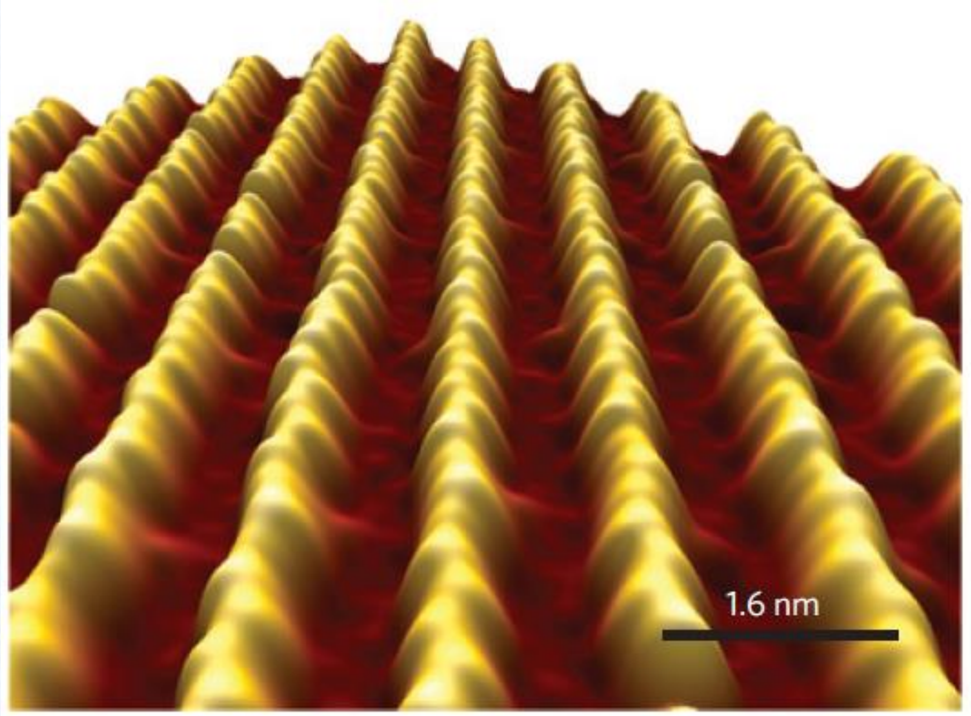


Interaction & geometry don't allow for 'quasi-free' motion:
collective excitations!

Spin- and charge degrees of freedom feel different influence:
Spin-Charge-Separation!



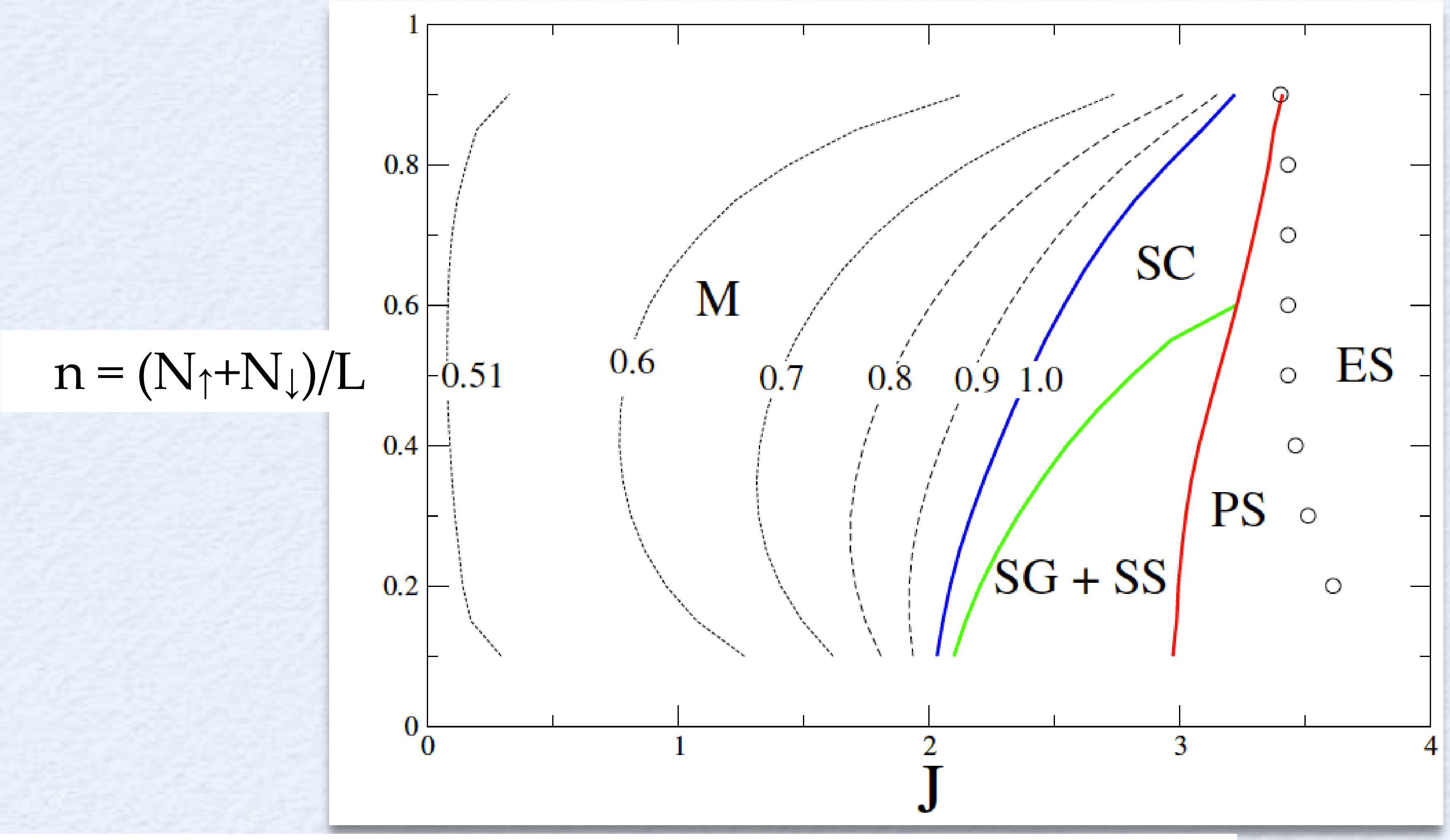
Experiments:



[C. Blumenstein et al., Nat. Phys. (2011)]

Phase diagram of the standard t-J-chain

$$\mathcal{H} = -t\sum_{i,\sigma}\left[c^\dagger_{i,\sigma}c_{i+1,\sigma} + h.c.\right] + J\sum_i\left(\vec{S}_i\cdot\vec{S}_{i+1} - \frac{1}{4}n_i n_{i+1}\right)$$



[A. Moreno, A. Muramatsu, and S.R. Manmana, PRB (2011)]

Two superconducting phases:

- low filling: K>1 + spin-gap ➥ Luther-Emery-liquid
- large filling: crossover from dominant density-density correlations to superconducting correlations

How does this translate to the t-$J_\perp$-chain, in particular in the presence of long-range interactions?

R. Manmana

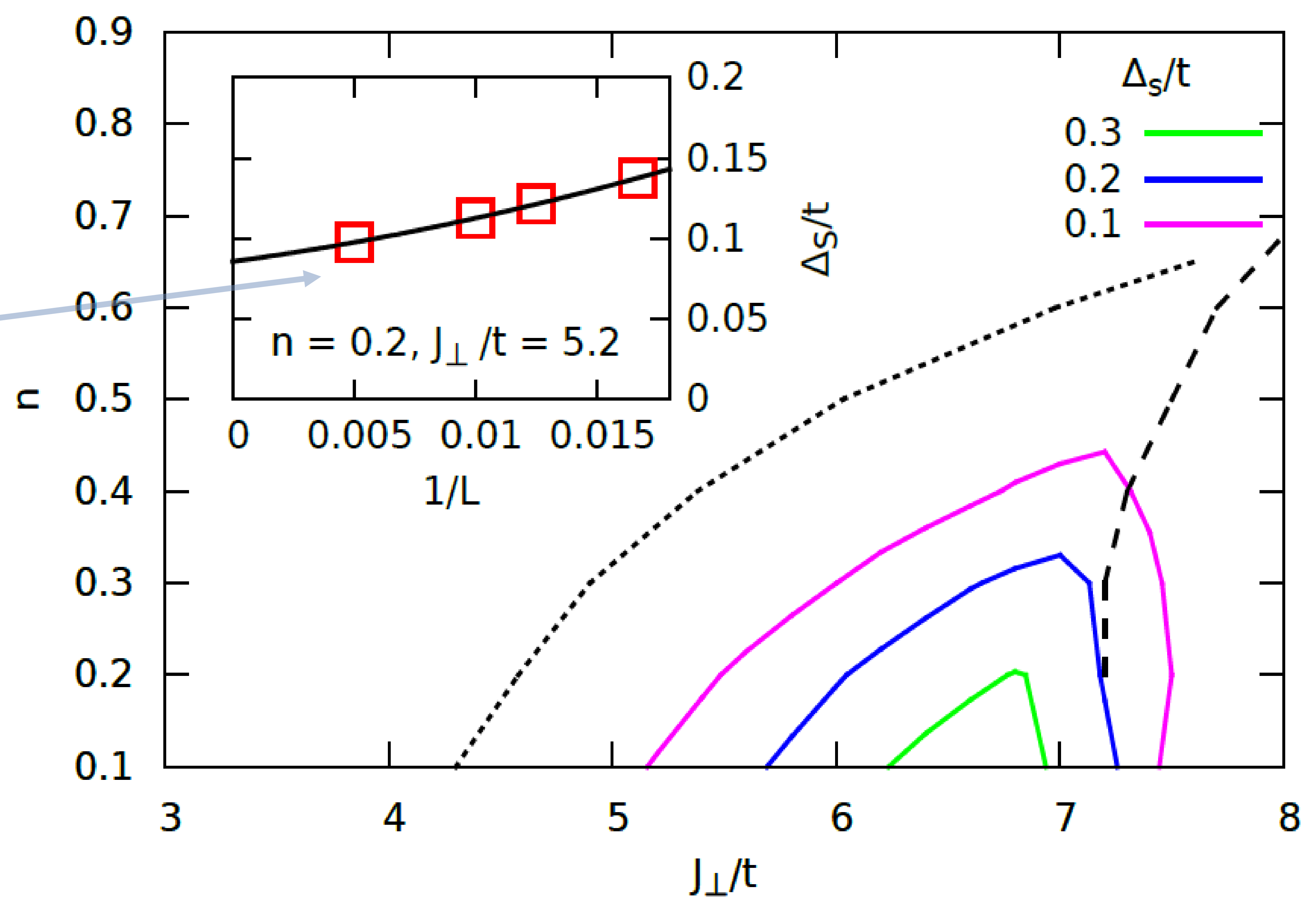
Phase diagram of the standard t-J-chain: How to obtain it?

[S.R. Manmana et al., PRA (2017)]

Spin gap:

$$\Delta_S = E_0(N, S^z_{\text{total}} = 1) - E_0(N, S^z_{\text{total}} = 0)$$

Finite-size extrapolation!



(similarly: inverse compressibility)

Phase diagram of the standard t-J-chain: How to obtain it?

[S.R. Manmana et al., PRA (2017)]

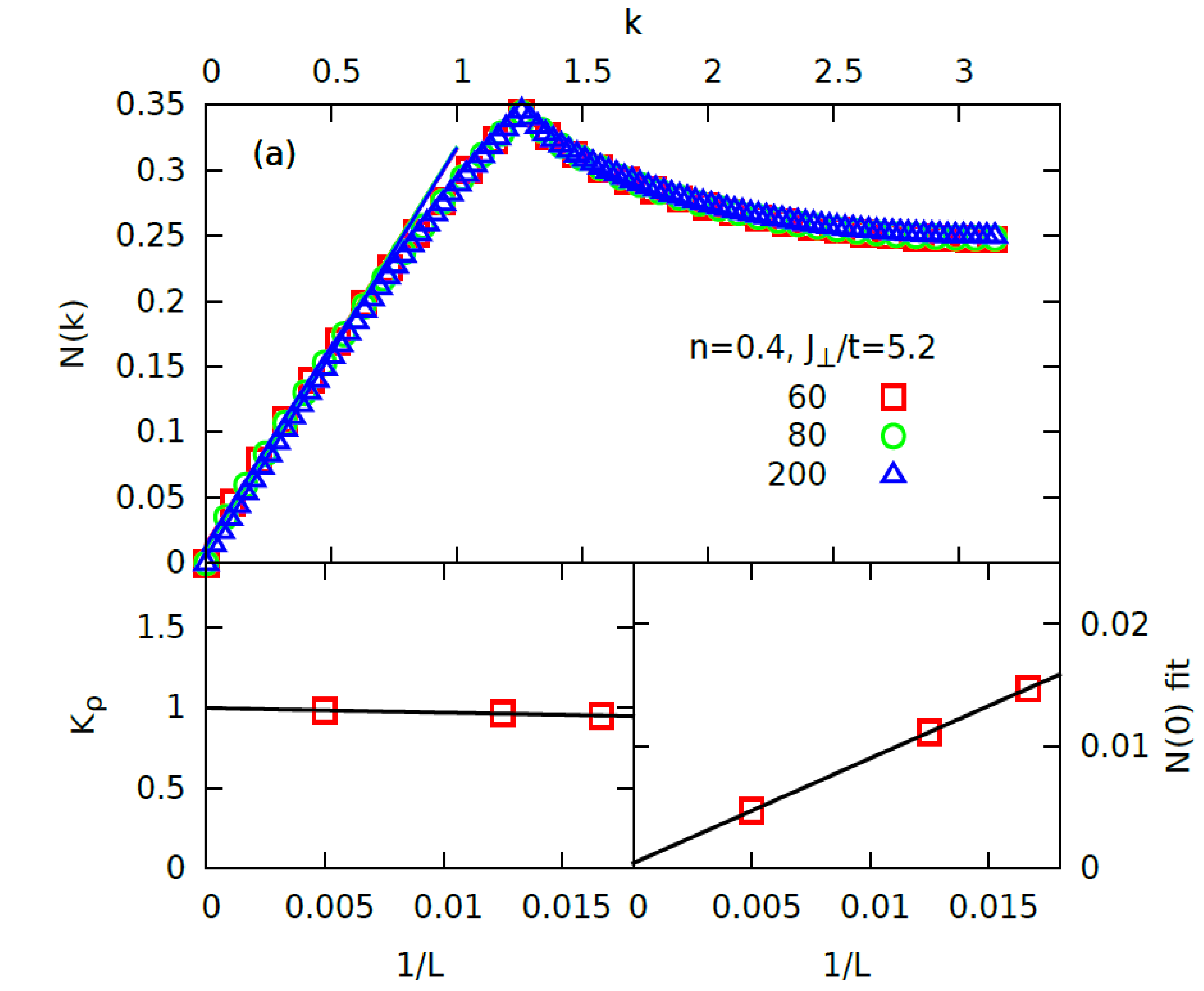
Luttinger parameter:
From structure factor

$$N(k) = \frac{1}{L}\sum_{i,j=1}^{L} e^{ik(i-j)} N_{ij}$$

with

$$N_{ij} = \langle n_i n_j \rangle - \langle n_i \rangle \langle n_j \rangle$$

$$N(k) \to K_\rho \frac{|k|}{\pi} \quad \text{for } k \to 0$$



Bosonization/ theory of Luttinger liquids:

No spin gap:

$$\langle n(r)n(0)\rangle = \frac{K_\rho}{(\pi r)^2} + A_1 \frac{\cos(2k_F r)}{r^{K_\sigma + K_\rho}} + A_2 \cos(4k_F r) r^{-4K_\rho}$$

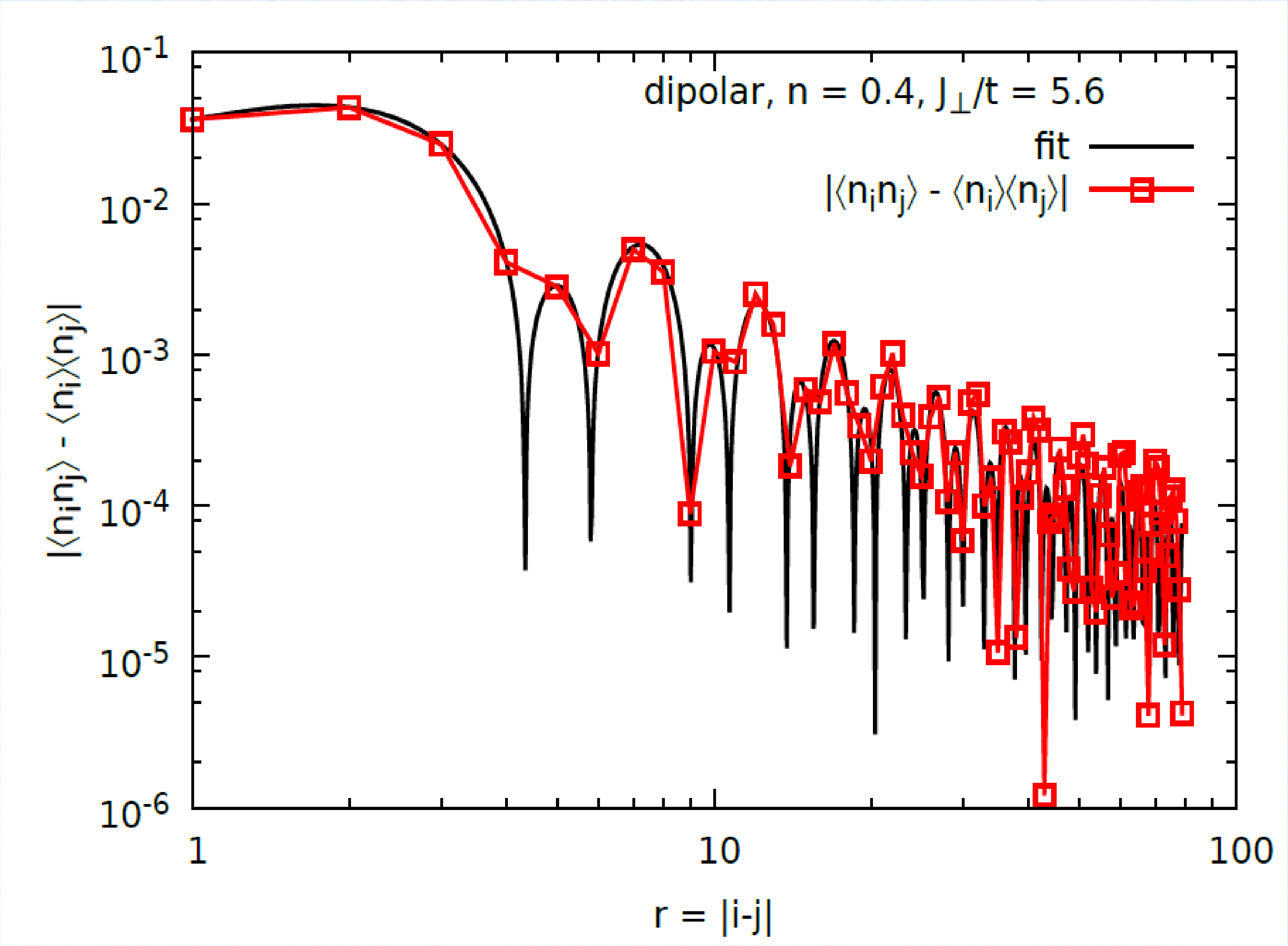
With spin gap:

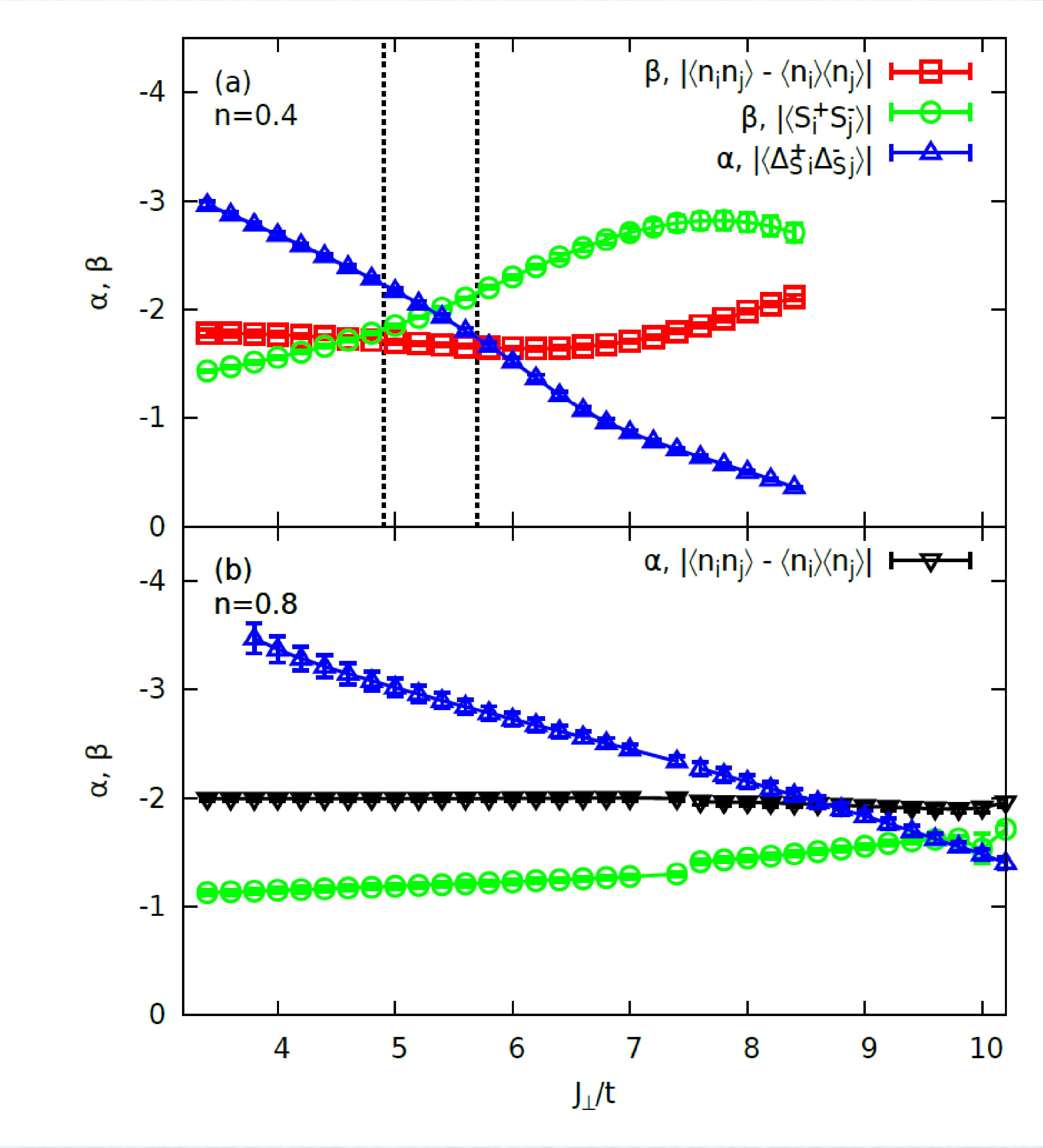
$$\langle n(r)n(0)\rangle = \frac{K_\rho}{(\pi r)^2} + A_1 \cos(2k_F r) r^{-K_\rho}$$

Phase diagram of the standard t-J-chain: How to obtain it?

[S.R. Manmana et al., PRA (2017)]

Dominant correlation functions:
fit and compare exponents

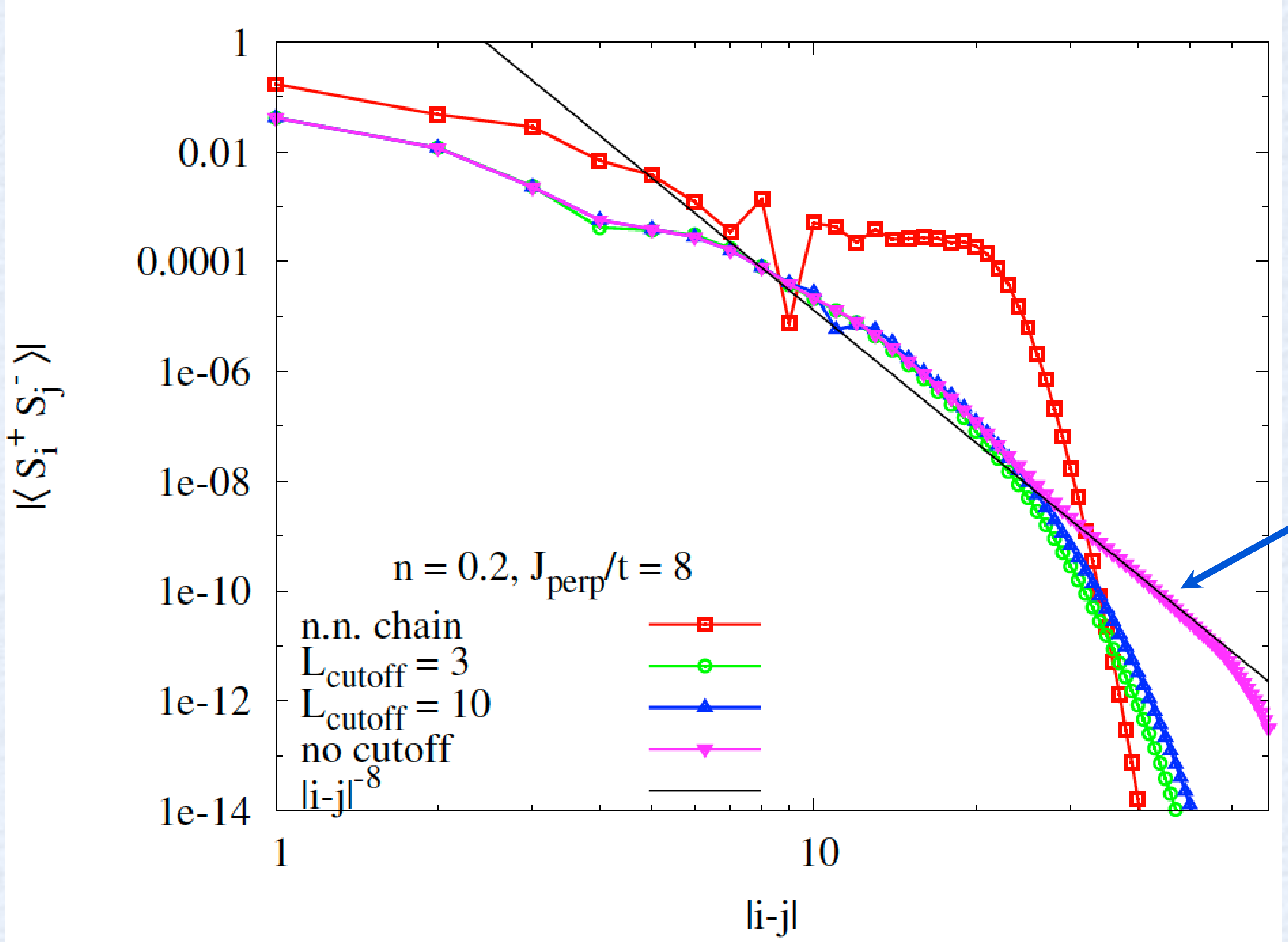




Effect of long-range interactions

[S.R. Manmana et al., PRA (2017)]

Spin gap: expect exponentially decaying correlations



Perturbation theory on dipolar Ising model:

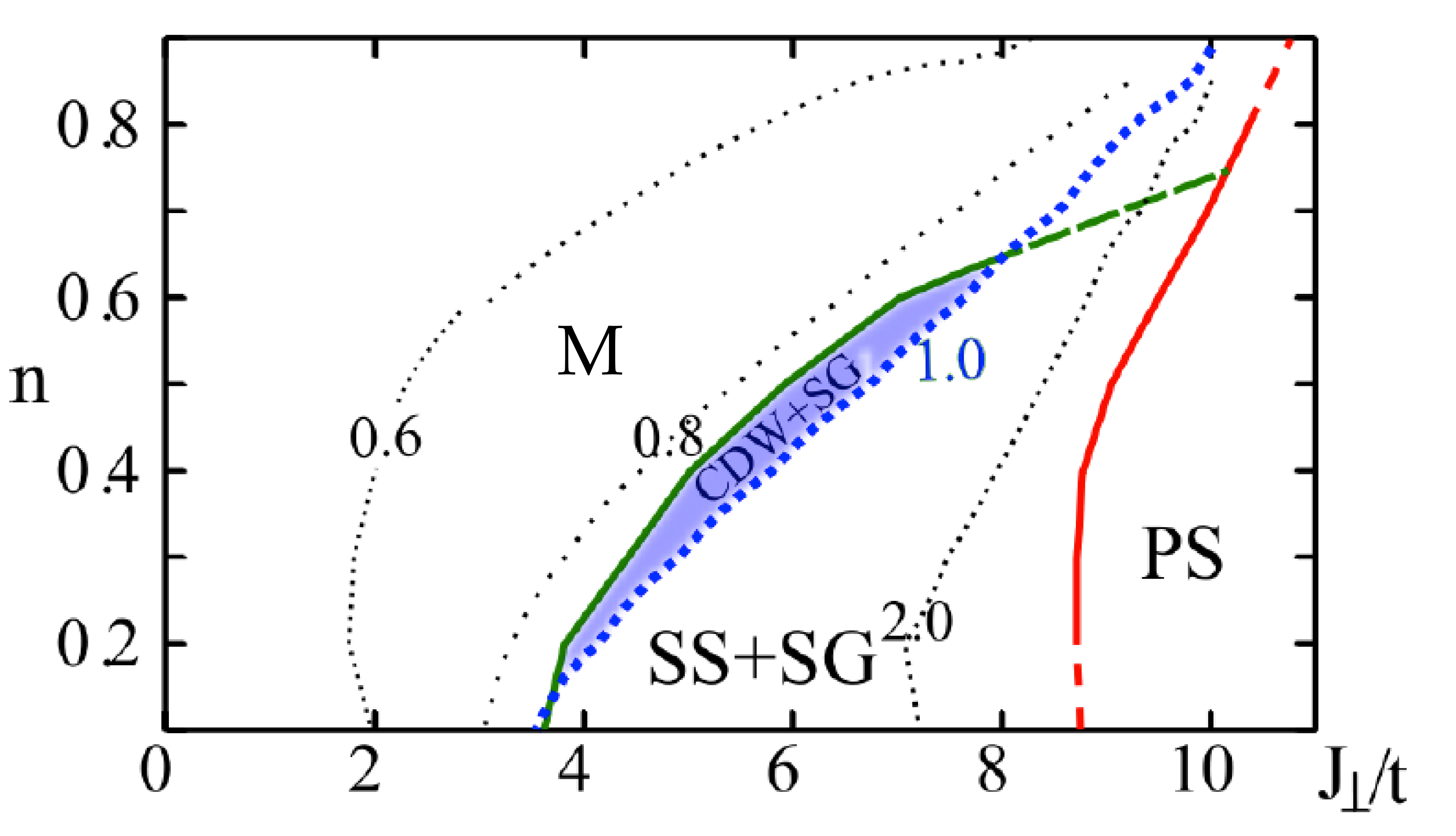
$$\langle S_i^+ S_j^- \rangle \;=\; -\frac{\lambda}{2} h(i,j) \frac{1}{|i-j|^3} \left(\frac{\delta_{i,j-1} + \delta_{i,j+1}}{8} + \frac{1}{8} \right)$$

Numerics for Ising models / proofs for Gaussian states:
[Deng et al., PRA **72**, 063407 (2005);
Schachenmayer et al., NJP **12** (2010) 103044;
Schuch et al., Comm. Math. Phys. **267**, 65 (2006)]

Phase diagram of the dipolar t-J⊥-chain

$$\mathcal{H} = -t\sum_{i,\sigma}\left(f^\dagger_{i,\sigma}f_{i+1,\sigma} + h.c.\right) + \frac{J_\perp}{2}\sum_{i,j}\frac{1}{|i-j|^3}\left(S_i^+S_j^- + S_i^-S_j^+\right)$$

[S.R. Manmana et al., PRA (2017)]



- similar to standard t-J-chain, broadened superconducting region
- $\Delta_S = 0$ and $K_\rho = 1$ lines interchange
  - ➠ additional CDW+SG-phase
- Spingap about 2x larger than in standard t-J-chain:
  - spin-anisotropy & long-ranged interactions ➠ stabilize superconducting phase

More unconventional states: 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:

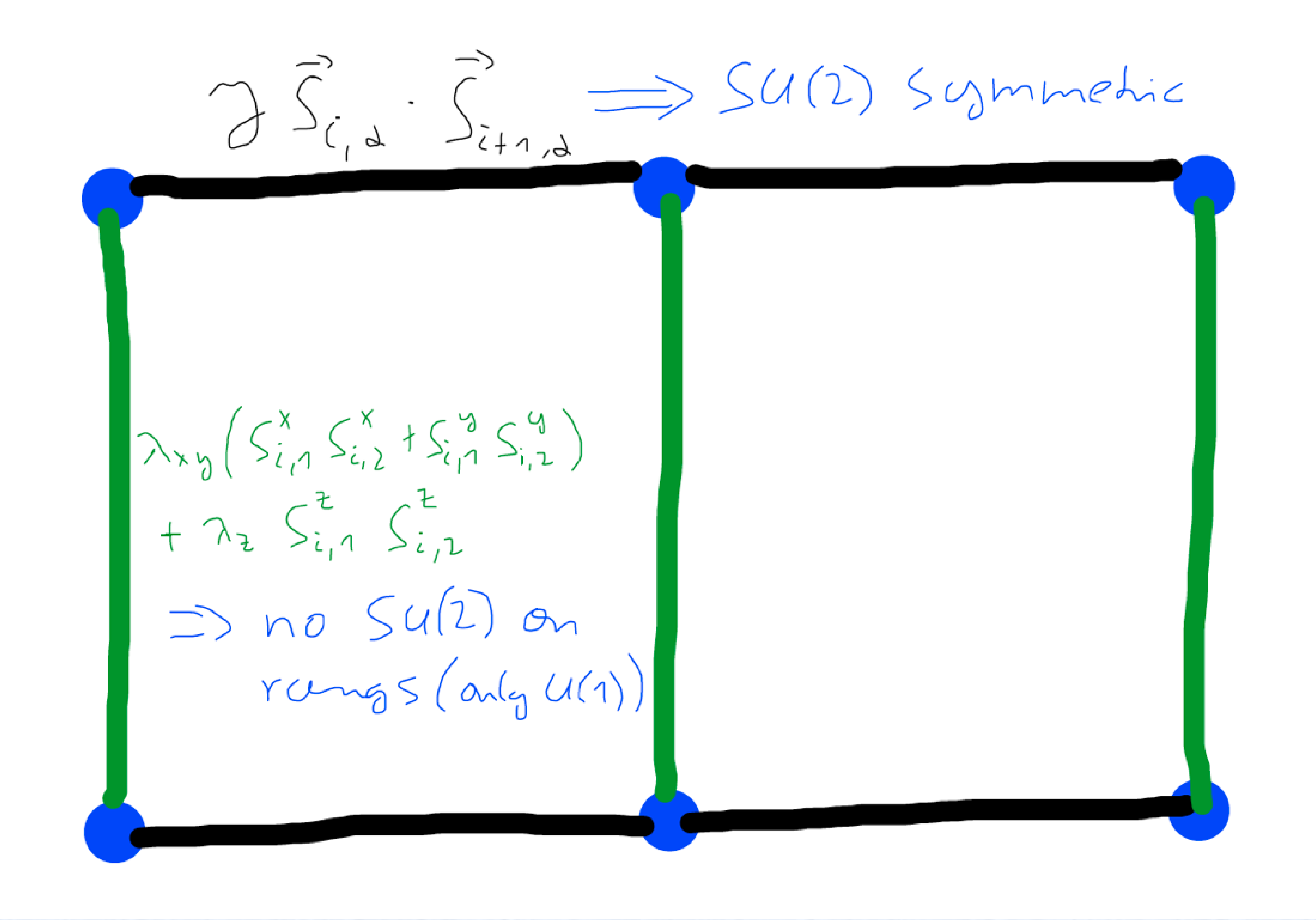
(a) distinct SPT states with a given symmetry cannot smoothly deform into each other without phase transition, if the deformation preserves the symmetry.

(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 $\vert\alpha\rangle_j$	B $\vert\beta\rangle_j$

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

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: $\Delta_S^0 = E_1(S^z_{\mathrm{total}} = 0) - E_0(S^z_{\mathrm{total}} = 0)$

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

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

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'

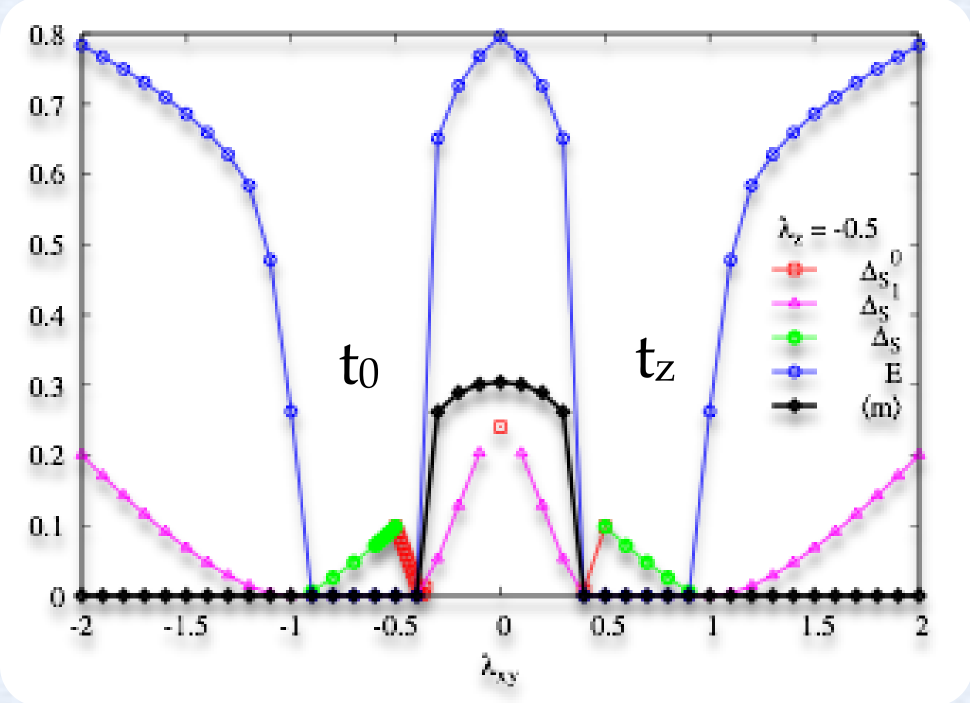
	R_z	R_x	σ	Active operators	SPT phases
E_0	1	1	1		Rung-singlet[a], $t_x \times t_x, \ldots$
E_1	I	$i\sigma_z$	σ_y	(S_-^z, S_+^z, SS_-)	$t_x \times t_y$
E_2	σ_z	I	$i\sigma_y$	(S_-^x, S_+^x, SS_-)	$t_y \times t_z$
E_3	$i\sigma_z$	σ_x	I	(S_+^x, S_+^y, S_+^z)	$t_0, t_x \times t_y \times t_z$
E_4	σ_z	$i\sigma_z$	$i\sigma_x$	(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 $$O_\pm = O_1 \pm O_2$$
$$SS_- = \vec{S}_{i,1} \cdot \vec{S}_{i+1,1} - \vec{S}_{i,2} \cdot \vec{S}_{i+1,2}$$

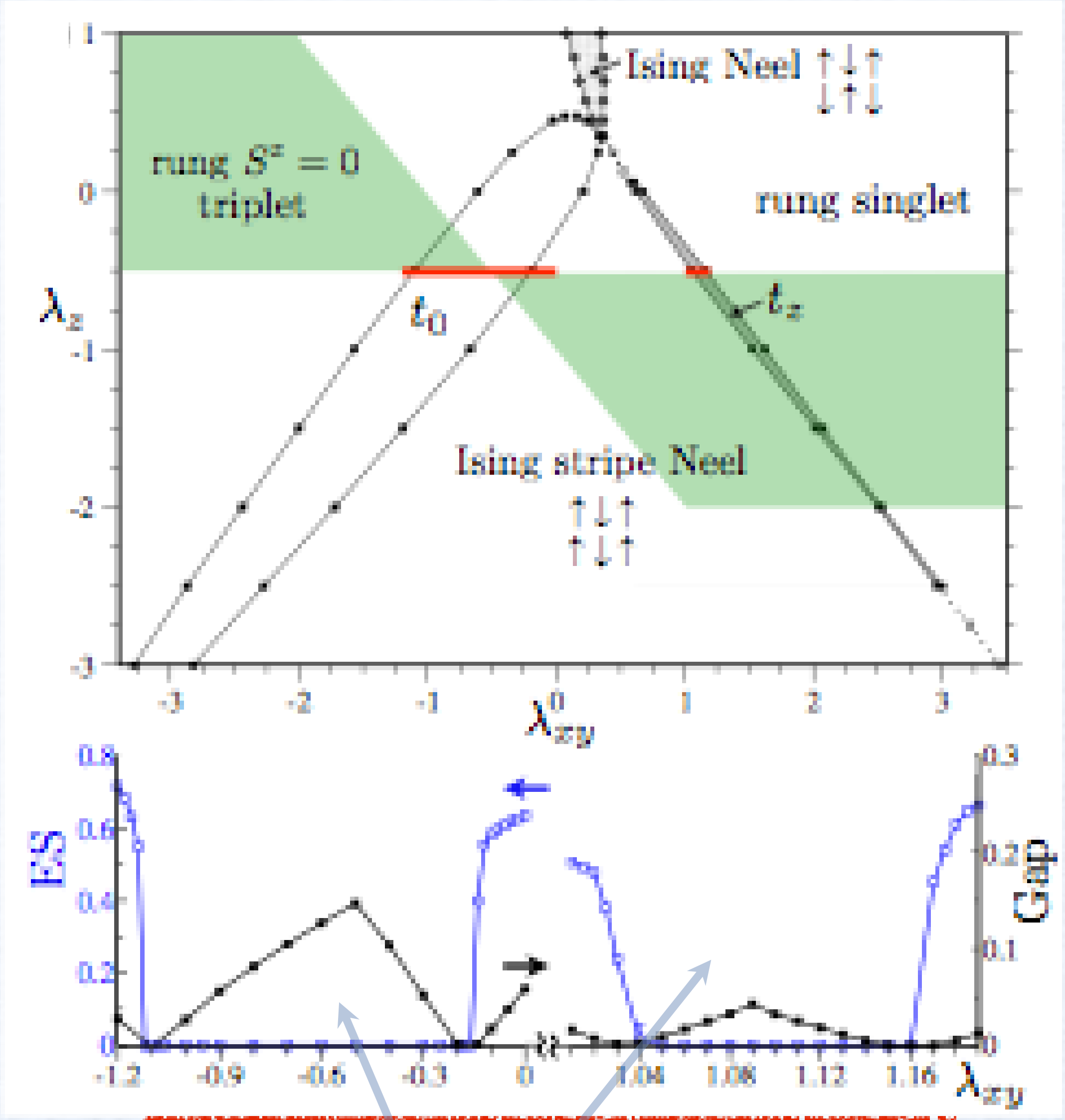
Phase Diagram without and with Long Range Interactions

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:

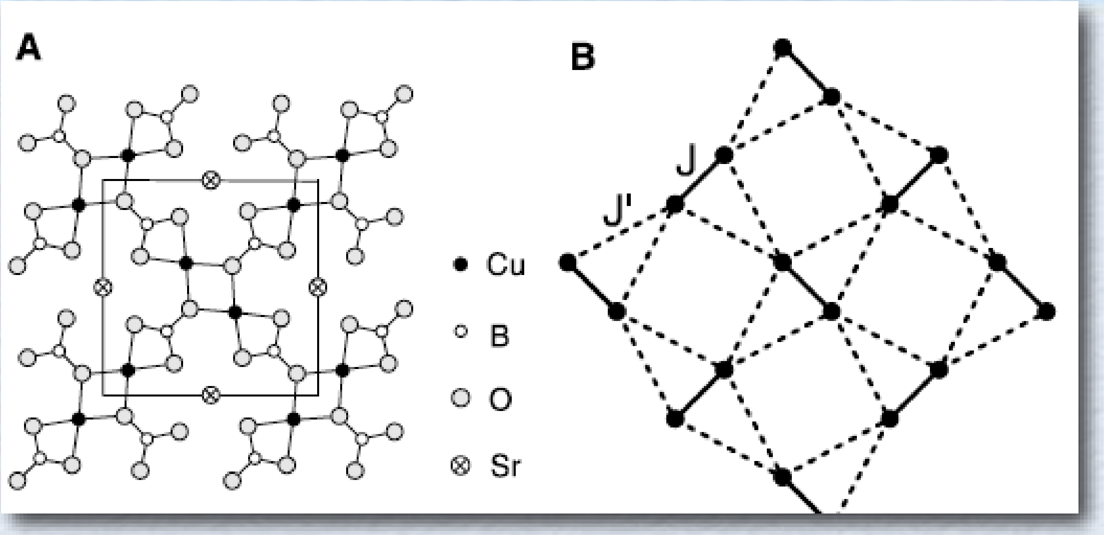
$S_1^x+S_2^x$:
E_0 = -188.24727291579
E_1 = -188.24727272182

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

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

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

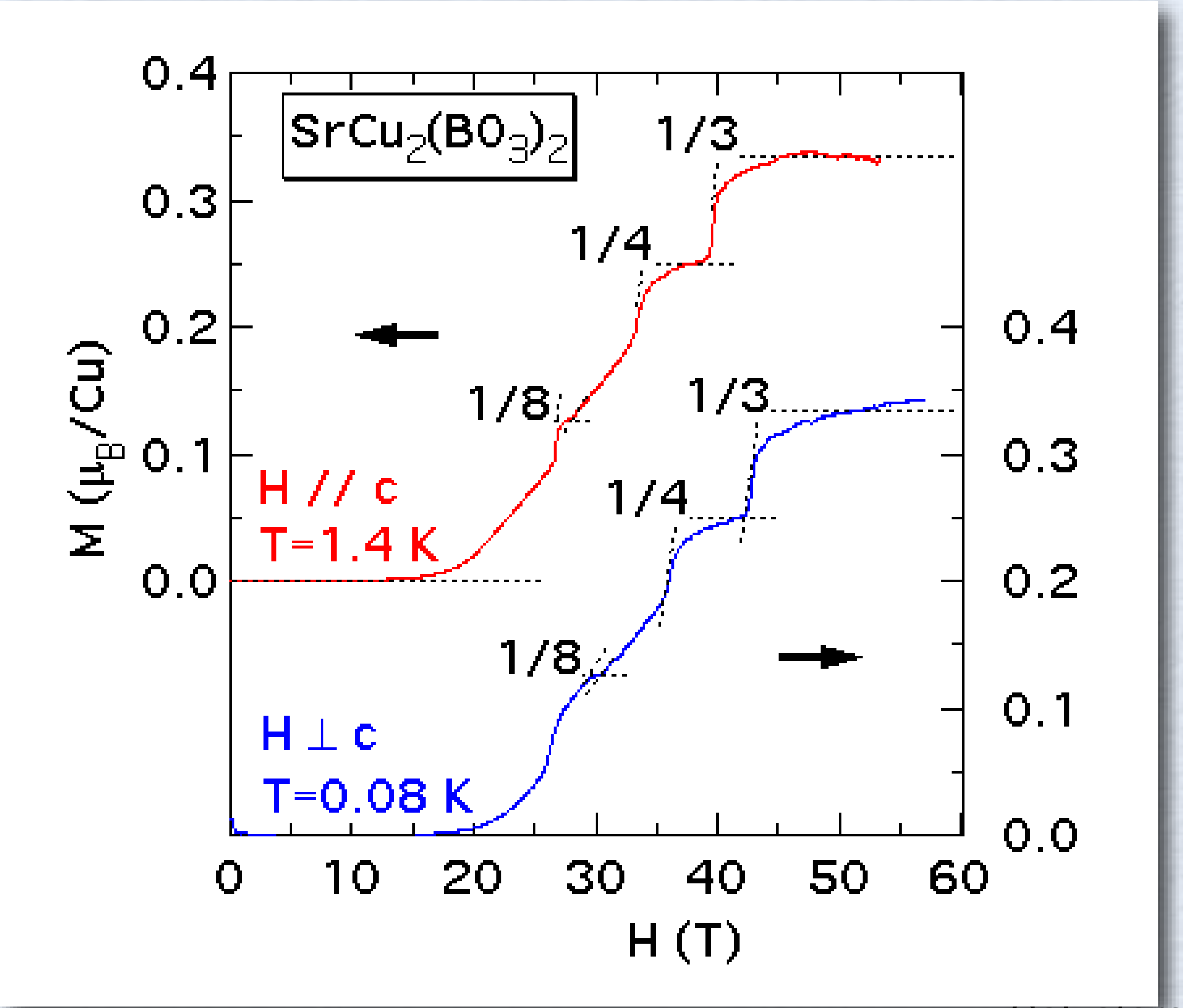
[H. Kageyama *et al.*, PRL **82**, 3168 (1999),
K. Kodama et al., Science **298**, 395 (2002)]



- 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



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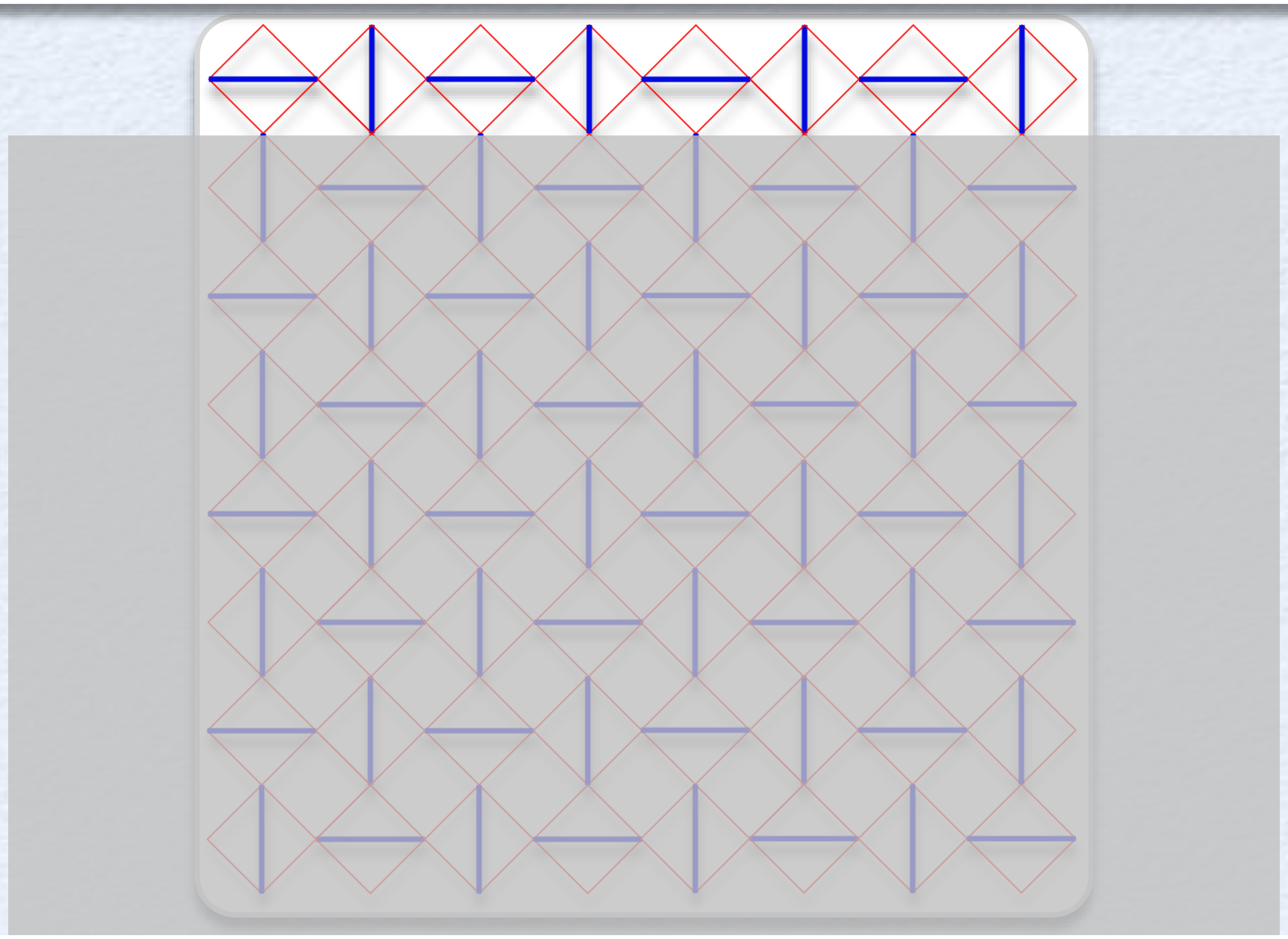
Shastry-Sutherland Lattice: From 1D to 2D

Heisenberg model on orthogonal dimer network:

$$\mathcal{H} = J \sum_{\ll i,j \gg} \vec{S}_i \cdot \vec{S}_j + J' \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j - H \sum_i S_i^z$$

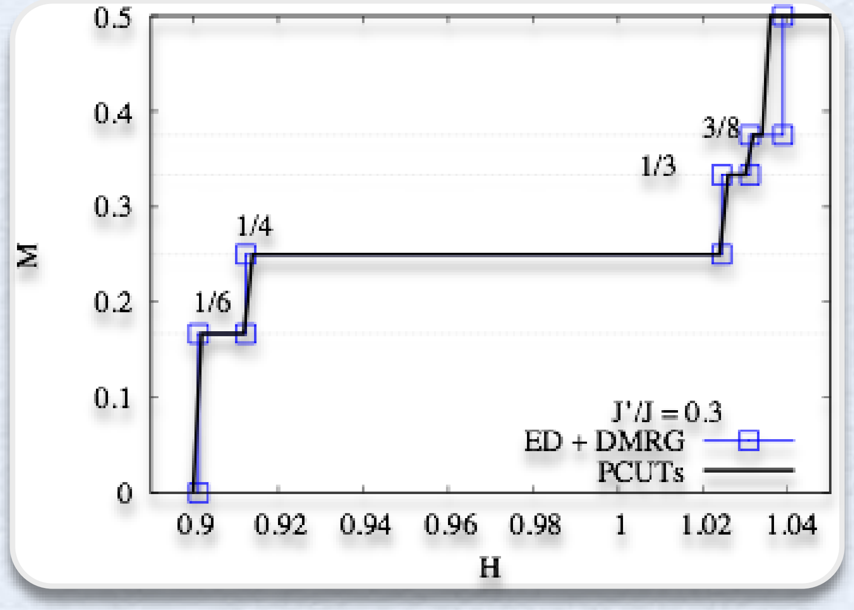


- 2D system: ground state at zero field is a product of singlets for J'/J << 1
- Full 2D system too difficult → take a stripe
- simplest stripe: 'orthogonal dimer chain' [Schulenburg & Richter, PRB 65, 054420 (2002)]
  infinite series of plateaux between M = 1/4 and 1/2
- 2 orthogonal dimer chains with transverse PBC: peculiar system, 'Shastry-Sutherland tube'
- crossover to 2D system: increase number of orthogonal dimer chains

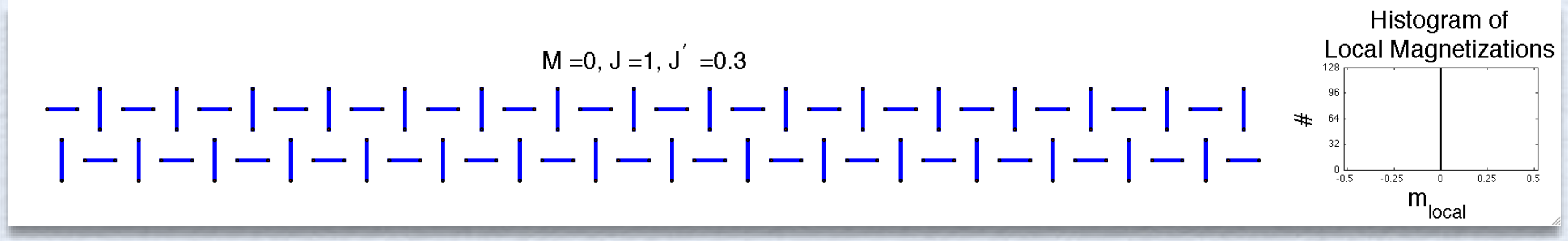
Quasi-1D version of the Shastry-Sutherland lattice: “2-leg Shastry-tubes”

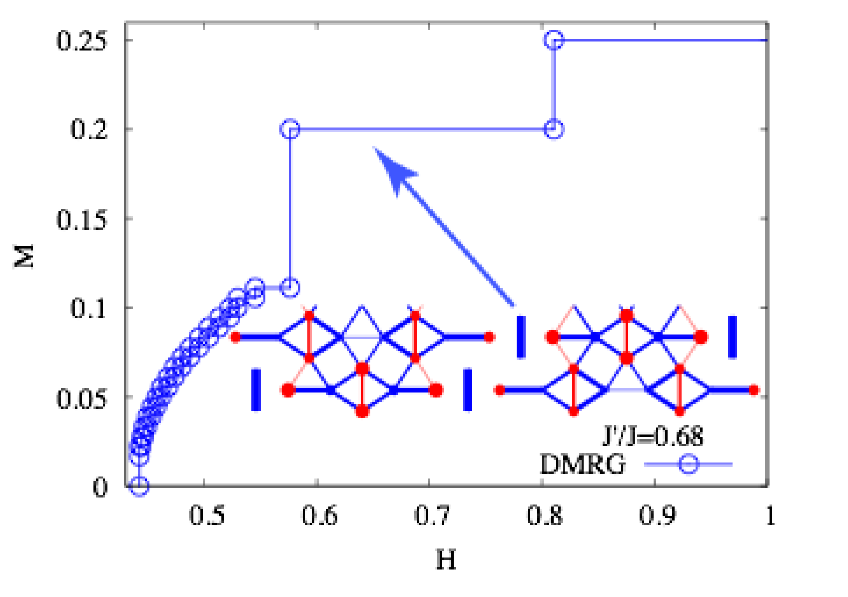
Magnetization curve: Compute ground state energies at different values of S^z_{total}
Do a Legendre-transform

[S.R. Manmana, J.-D. Picon, K.P. Schmidt, and F. Mila, EPL **94**, 67004 (2011)]

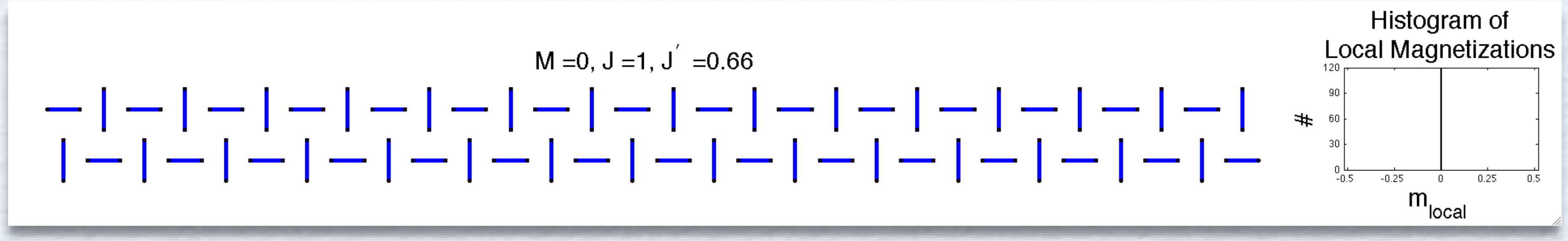


J’/J = 0.3 (“perturbative regime”)





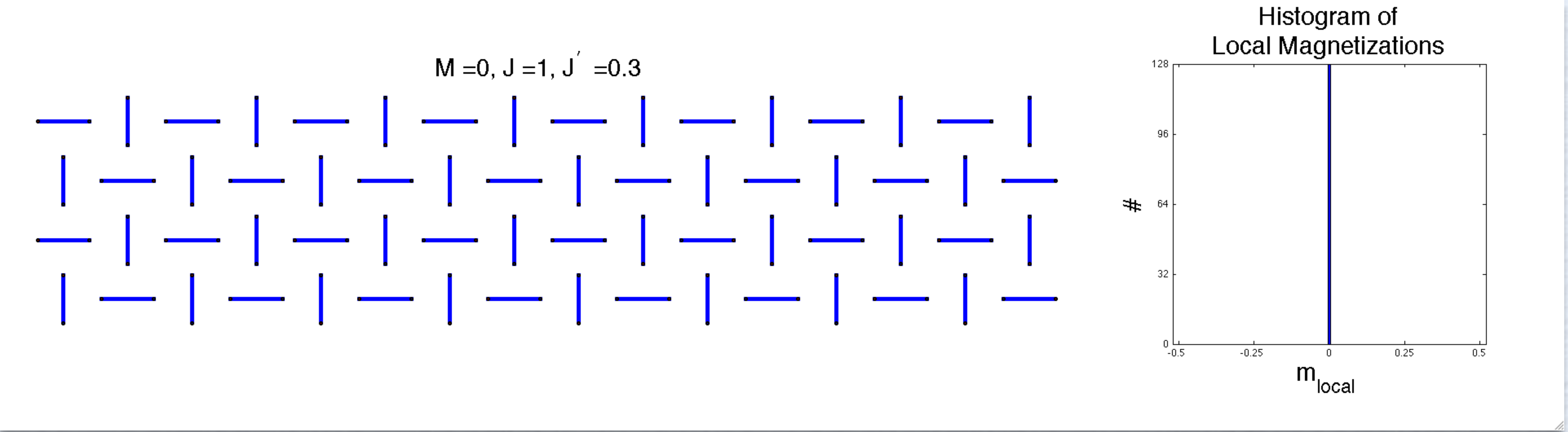
J’/J = 0.66 (“intermediate regime”)

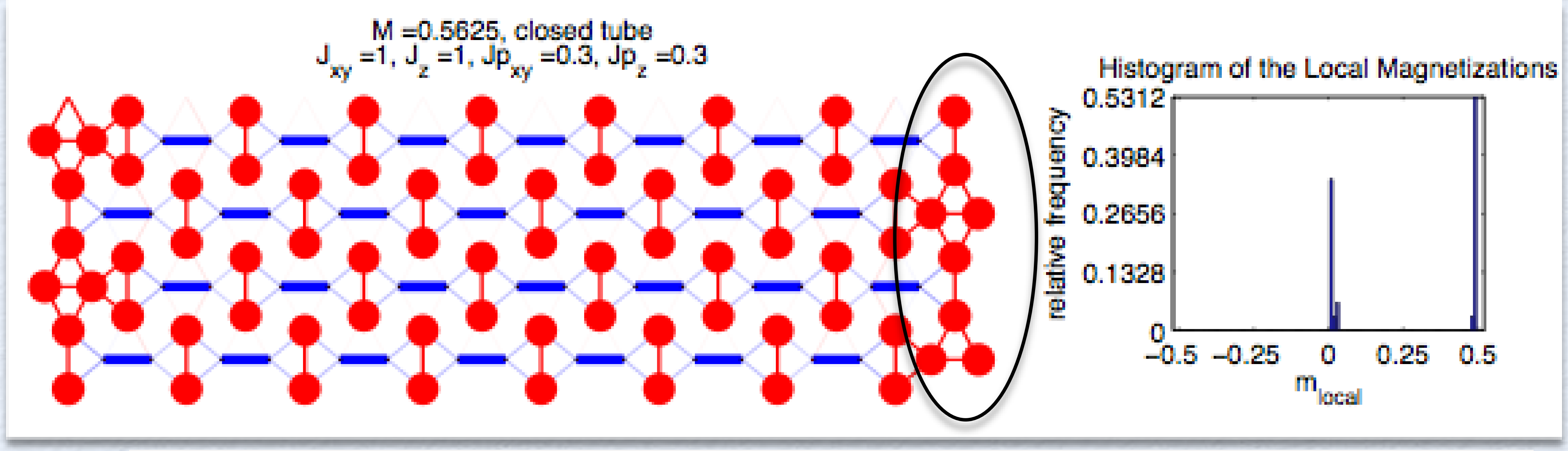


➥ Magnetization plateau of *bound states* of triplons

➟ *Qualitative* change of elementary building blocks: single triplons ➞ multi-triplon bound states

Quasi-2D version of the Shastry-Sutherland lattice: "4-leg Shastry-tubes"





- Excited states by injecting triplons, but fluctuations much more pronounced
- Periodic patterns of triplons: magnetization plateaux?
- At boundaries: emerging 1D structures?

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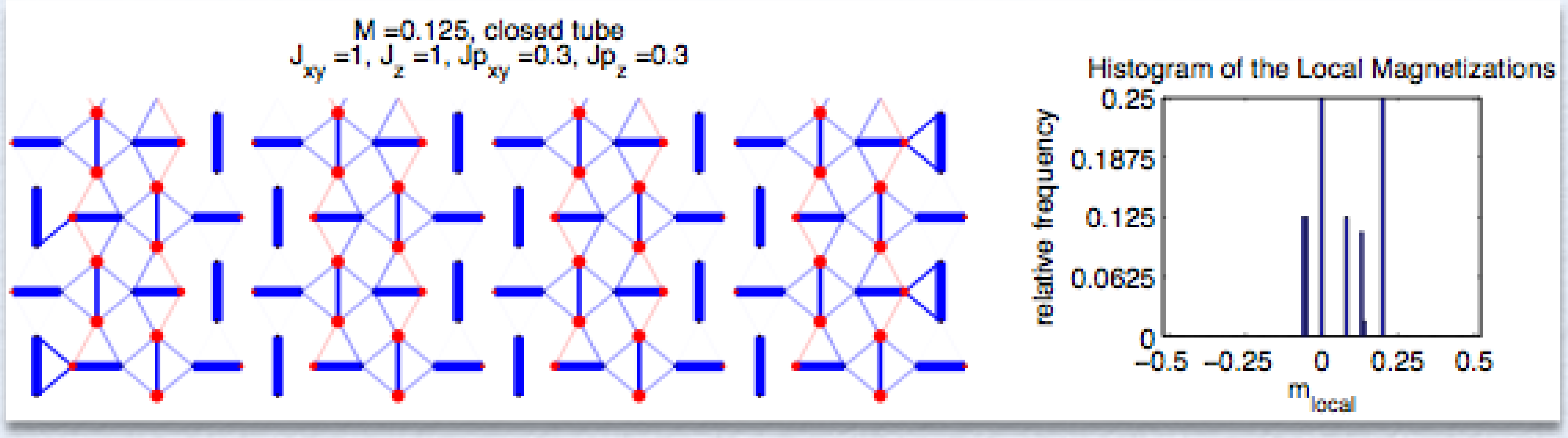
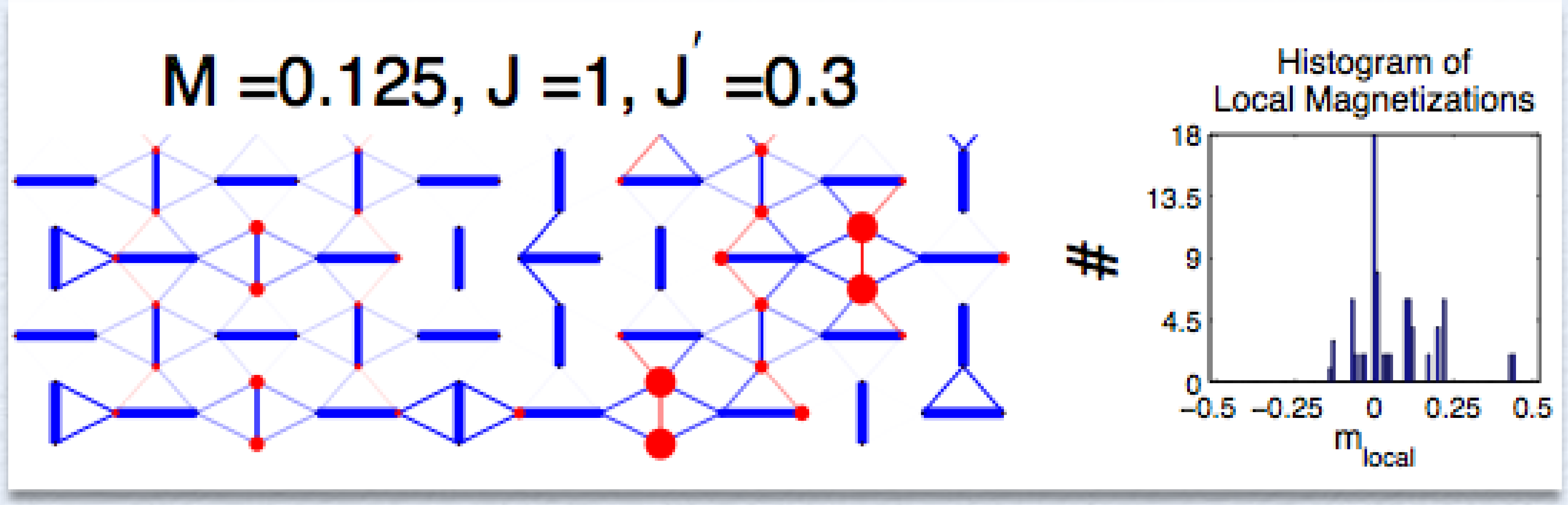
Quasi-2D Shastry-Sutherland lattice: DMRG on the 1/8 plateau



E/N = -0.319238530384945



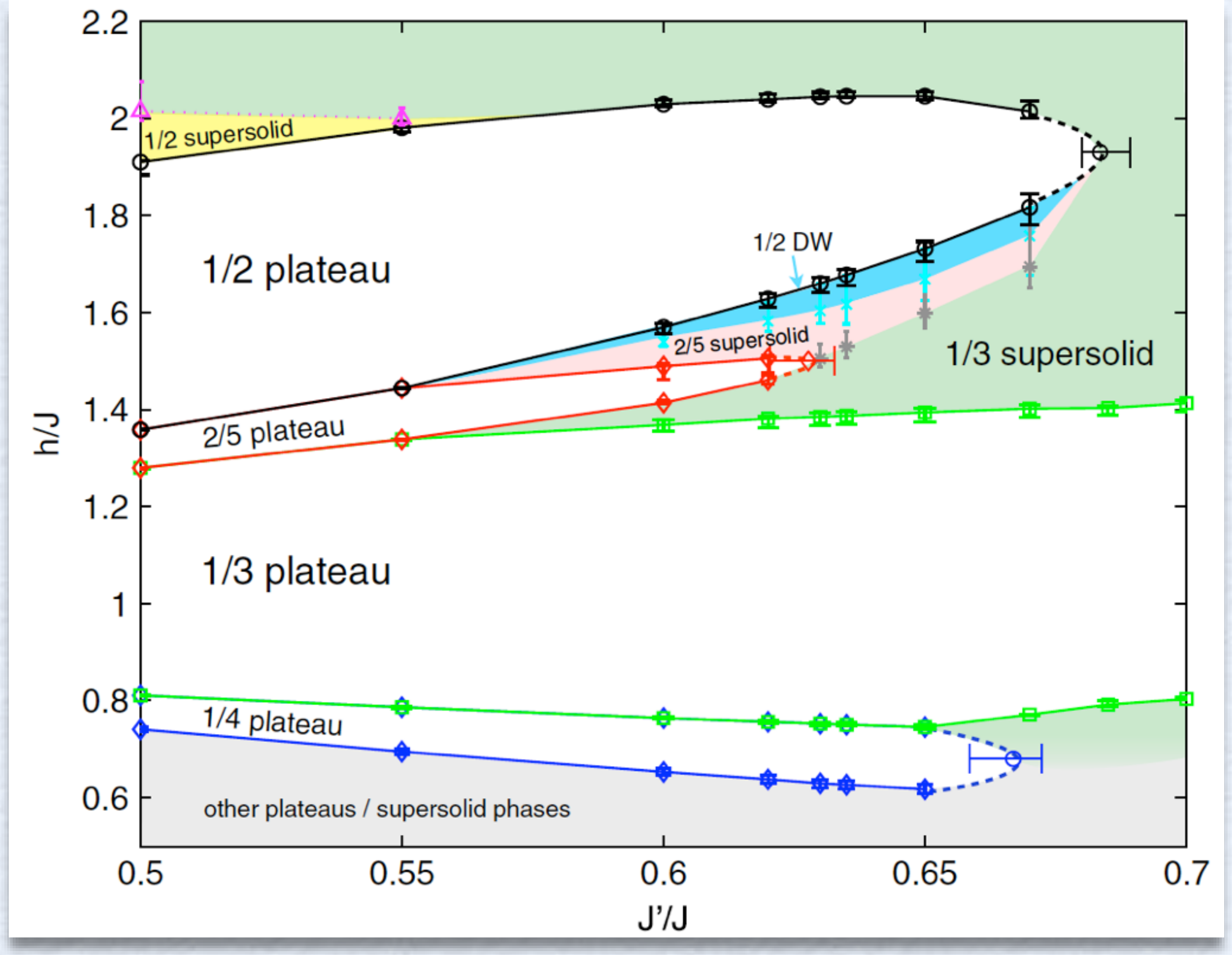
E/N = -0.319179928025625

Difference in E/N: only 6e-5 !!!

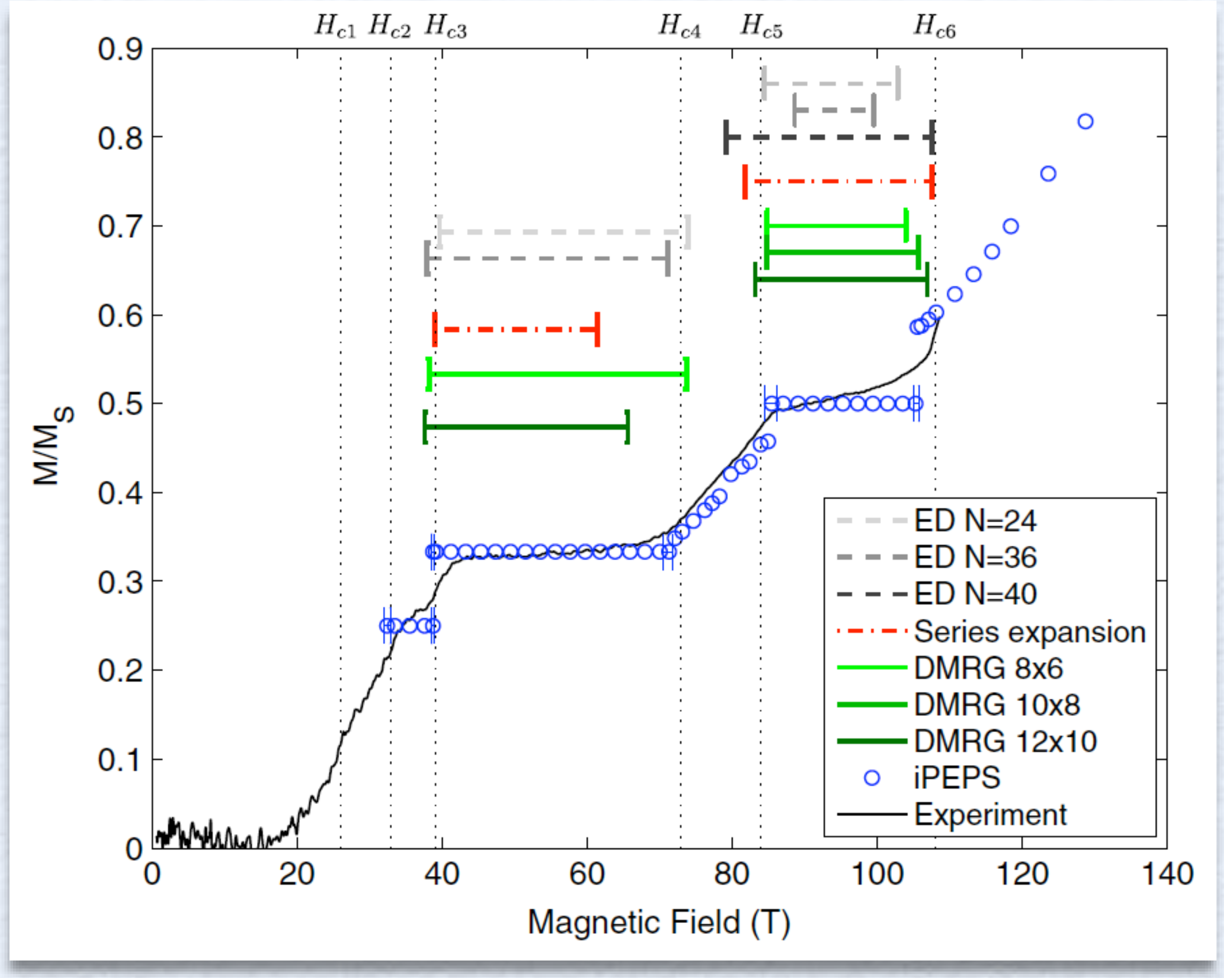
[S. White on Kagome: difference between VBC and spin-liquid ≈ 1e-3]

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)]

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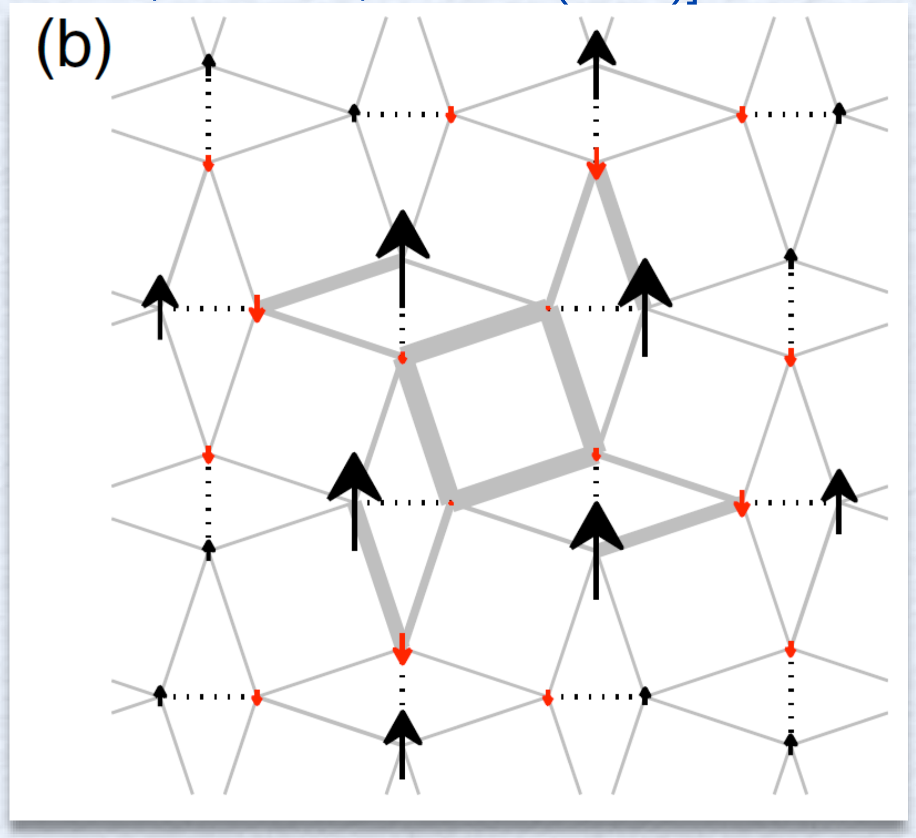
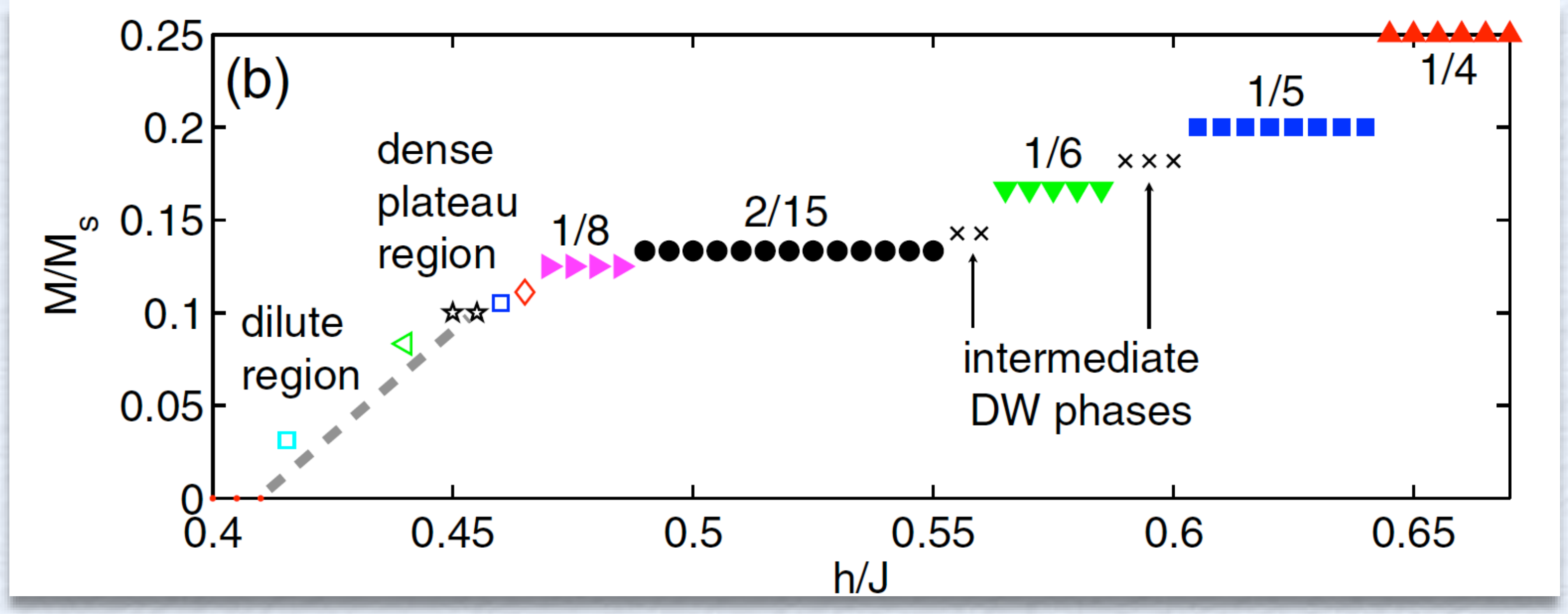
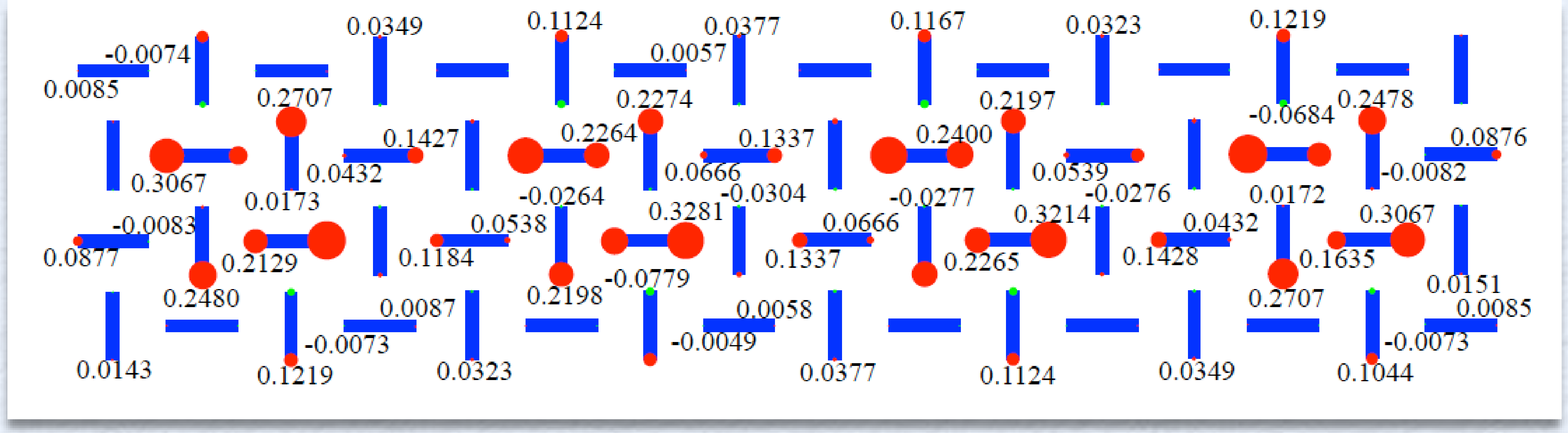
Approaching the 2D Shastry-Sutherland lattice: 2-triplon bound states & "pinwheel structure"

iPEPS: [P. Corboz and F. Mila, PRL **112**, 147203 (2014)]





DMRG with OBC: [G.R. Foltin, S.R. Manmana, and K.P. Schmidt, PRB **90**, 104404 (2014)]



"Numerically Exact Dynamics": Iterative Diagonalization

[S.R. Manmana *et al.*, AIP (2005)]

Lanczos procedure:
(Krylov space method)

K. Lánczos (1950)

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

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

Tridiagonalization of Hamiltonian matrix:

$$\mathbf{T}_n = \begin{pmatrix} a_0 & b_1 & & & \\ b_1 & a_1 & b_2 & \mathbf{0} & \\ & b_2 & a_2 & \ddots & \\ & \mathbf{0} & \ddots & \ddots & b_n \\ & & & b_n & a_n \end{pmatrix}$$

Projection of time evolution operator:
T.J. Park and J.C. Light, J. Chem. Phys (1986)

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

Error estimate:
M. Hochbruck and C. Lubich, SIAM (1997)

$$\begin{aligned} \varepsilon_n \;&:=\; \| \hat{U}|\psi\rangle - \hat{U}_{\text{approx}}|\psi\rangle \| \\ &\leq\; 12\,\exp\left\{-\frac{(w\,\Delta\tau)^2}{n}\right\}\left(\frac{e\,w\,\Delta\tau}{n}\right)^n, \; n \geq 2\,w\,\Delta\tau \end{aligned}$$

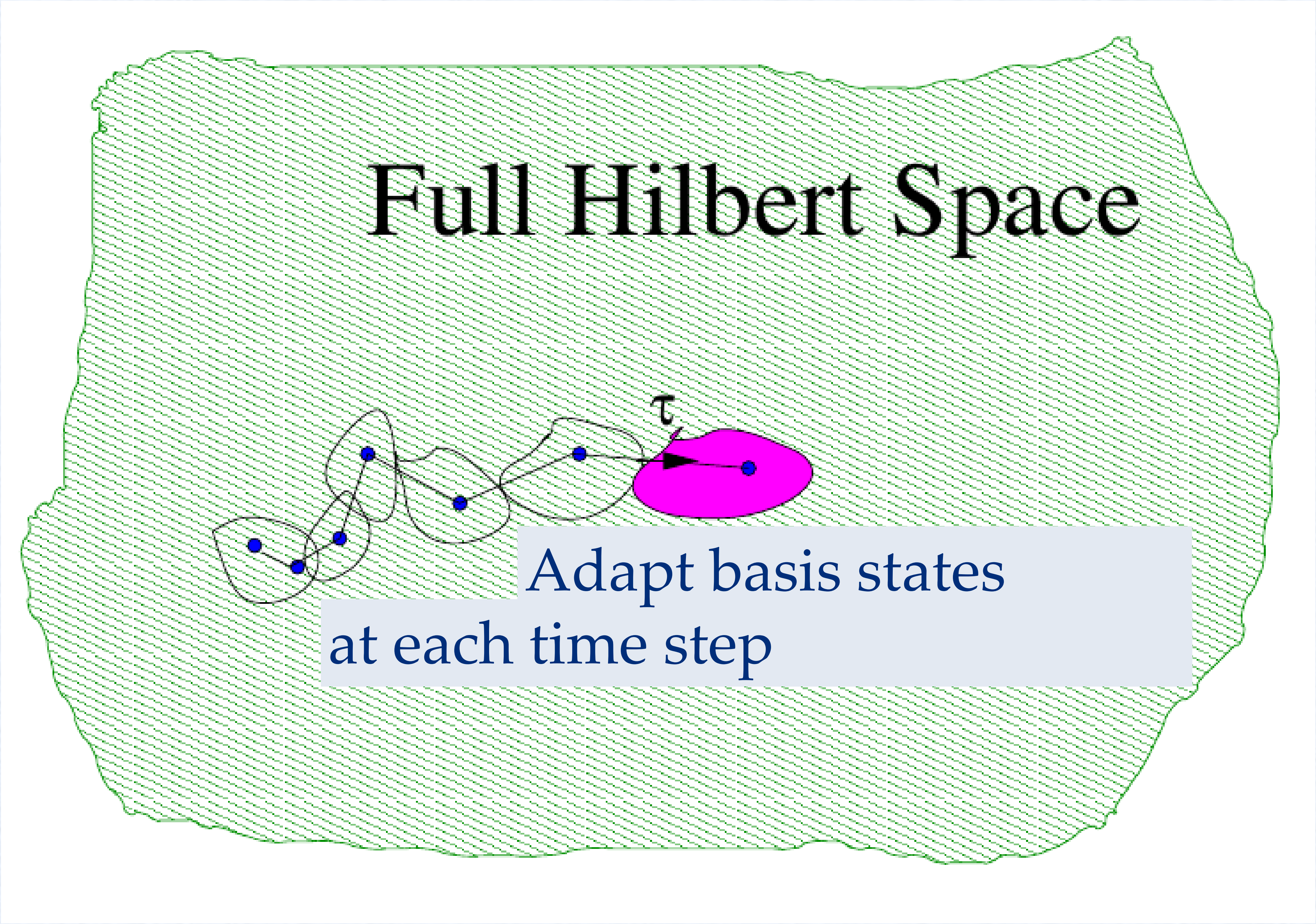
Usually n < 20 is sufficient

Larger systems possible

Pro's/Con's similar to 'full diagonalization'

➠ Need to store n vectors with dimension of H ☹

Time evolution with Matrix Product States

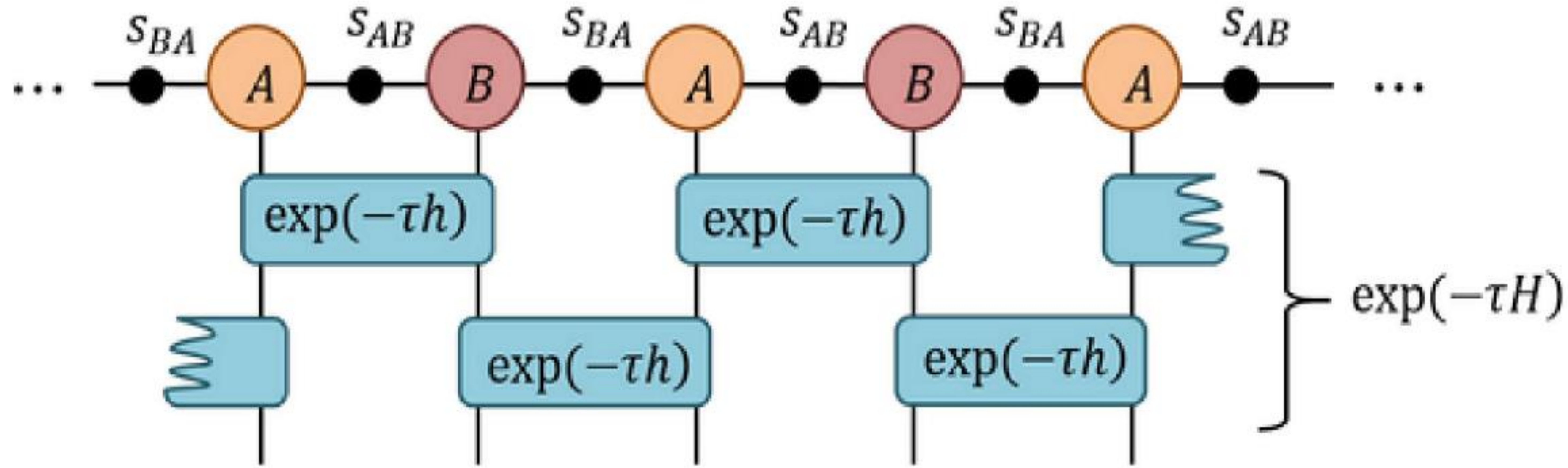


Time evolution with Matrix Product States: Trotter approach

Trotter decomposition:

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

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)

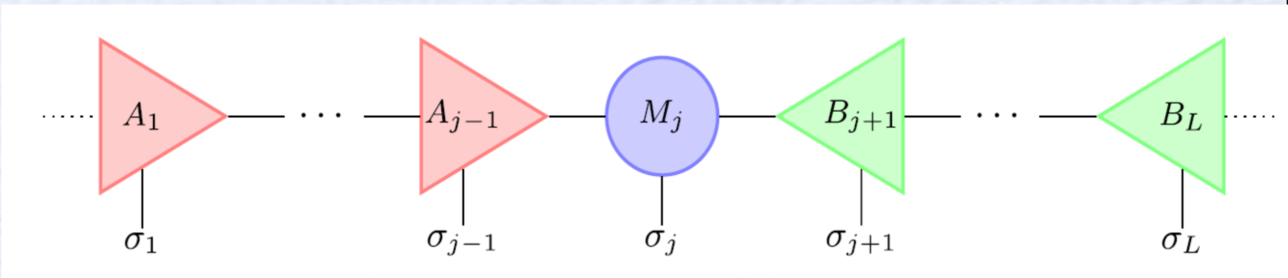
$$e^{-i\Delta\tau/\hbar\,\hat{H}}\,|\psi(\tau)\rangle \approx \mathbf{V}_n(\tau)\,e^{-i\Delta\tau/\hbar\,\mathbf{T}_n(\tau)}\,\mathbf{V}_n^+(\tau)\,|\psi(\tau)\rangle$$

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

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

Very versatile, arbitrary range interactions & geometries possible
Two variants:

- „global Krylov method“:
  perform all operations without taking into account MPS structure – costly!!!
- „local Krylov method“:
  apply Lanczos-projection while ‚sweeping‘
  through the system – sequentely updates A-matrices
  (problem: what about the remaining ones?)



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

MPO based time evolution

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

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

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

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

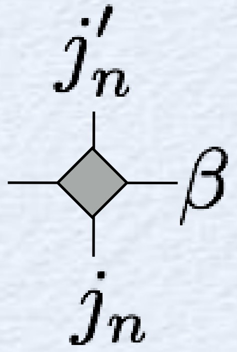
Neglect overlapping terms in expansion

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

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

Compact matrix product operator representation

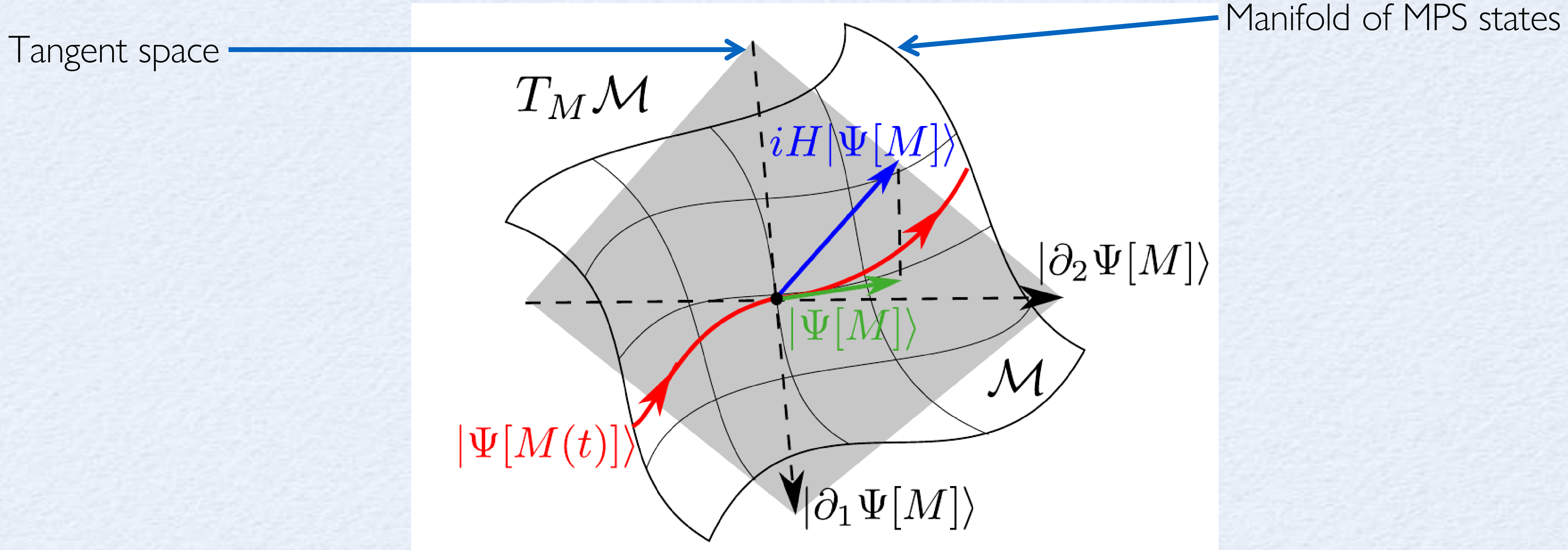
$$W^{[n]j_n j_n'}_{\alpha\beta} = \alpha$$



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

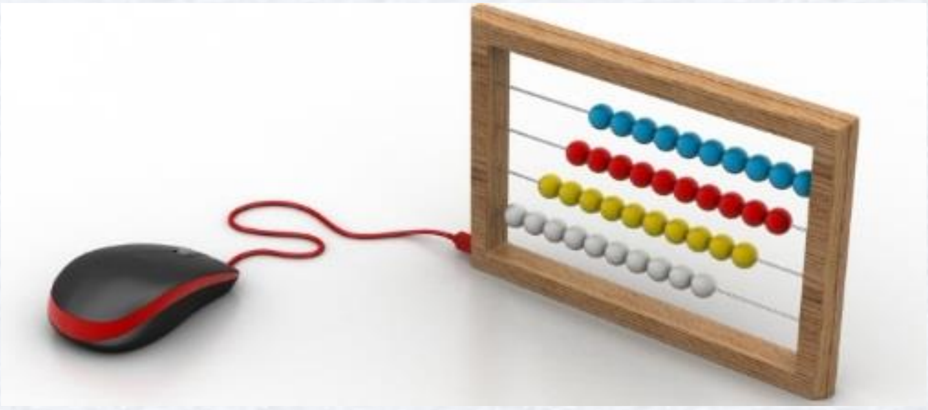
[J. Haegeman et al, arXiv:1408.5056]

Basic idea of TDVP:



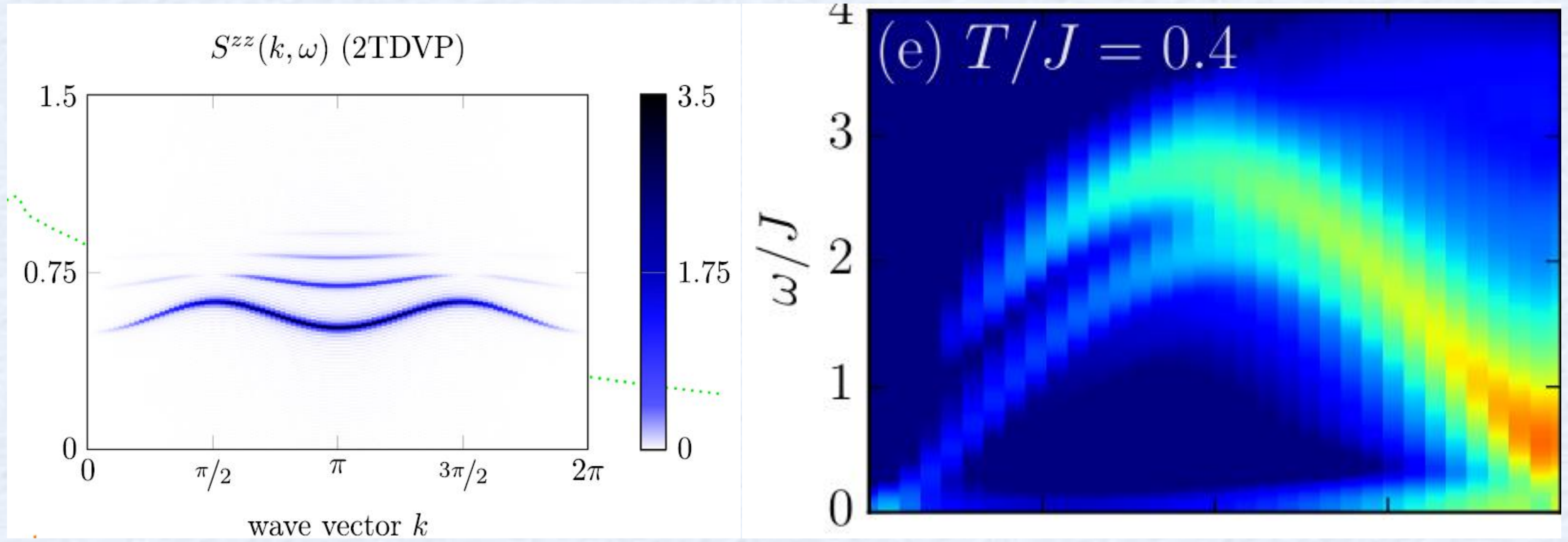
Projection onto tangent Space to MPS manifold: $$\frac{\mathrm{d}|\Psi[M]\rangle}{\mathrm{d}t} = -iP_{T_{|\Psi[M]\rangle}\mathcal{M}_{\mathrm{MPS}}}H|\Psi[M]\rangle$$ ⇒ Corrects/improves „local Krylov“ method

Part III: Dynamics
Spectral Functions and Full Time Evolution

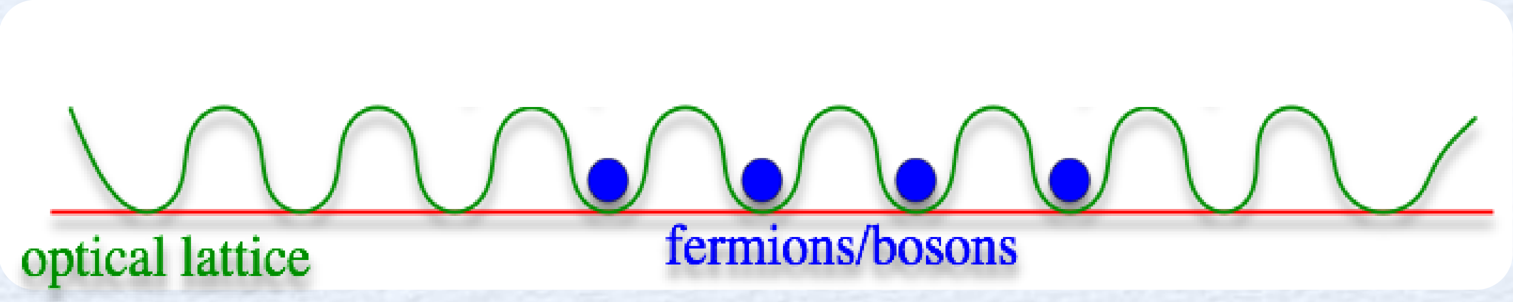


Examples

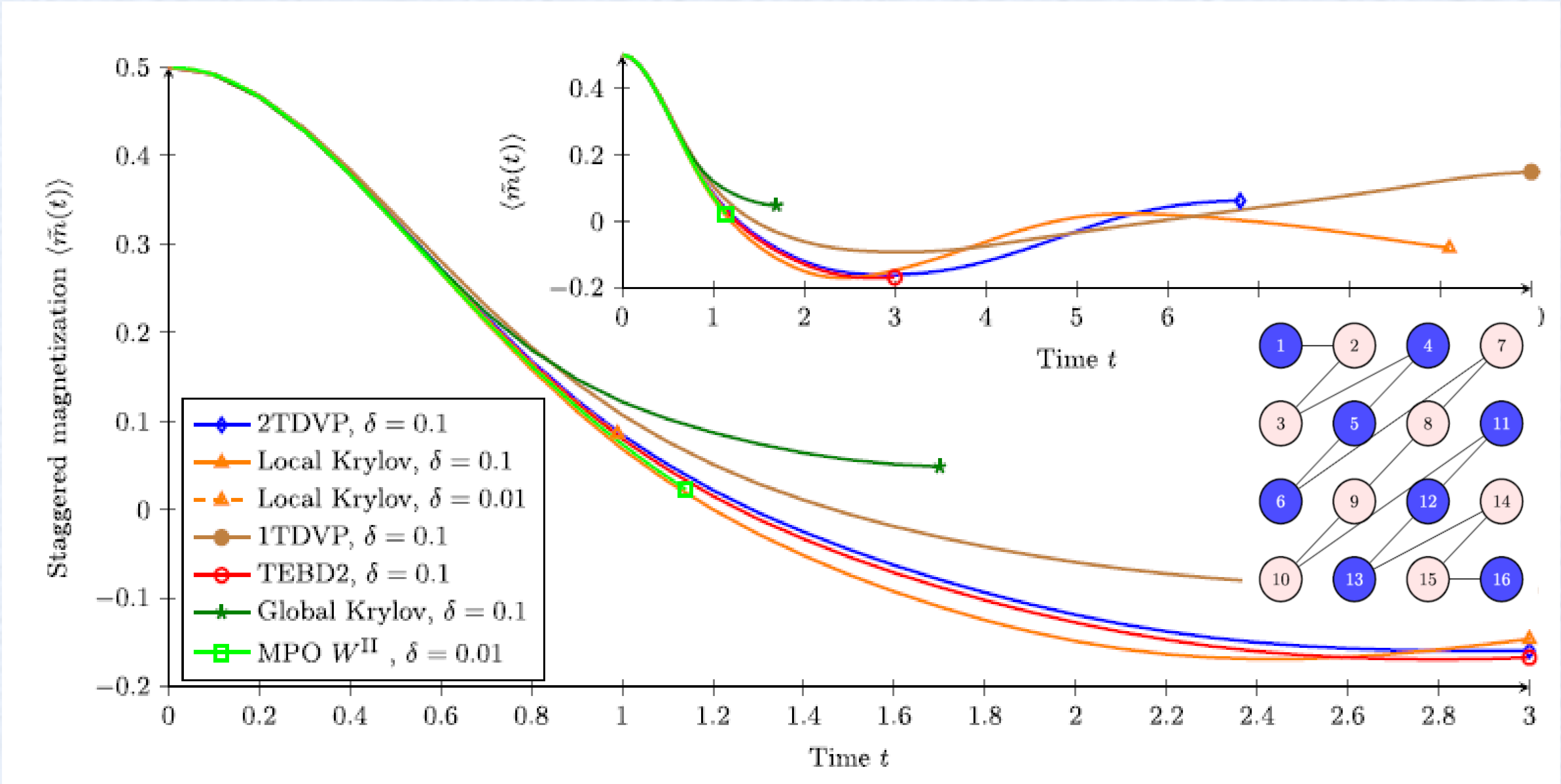
Dynamical spectral functions (also finite T, nonequilibrium)



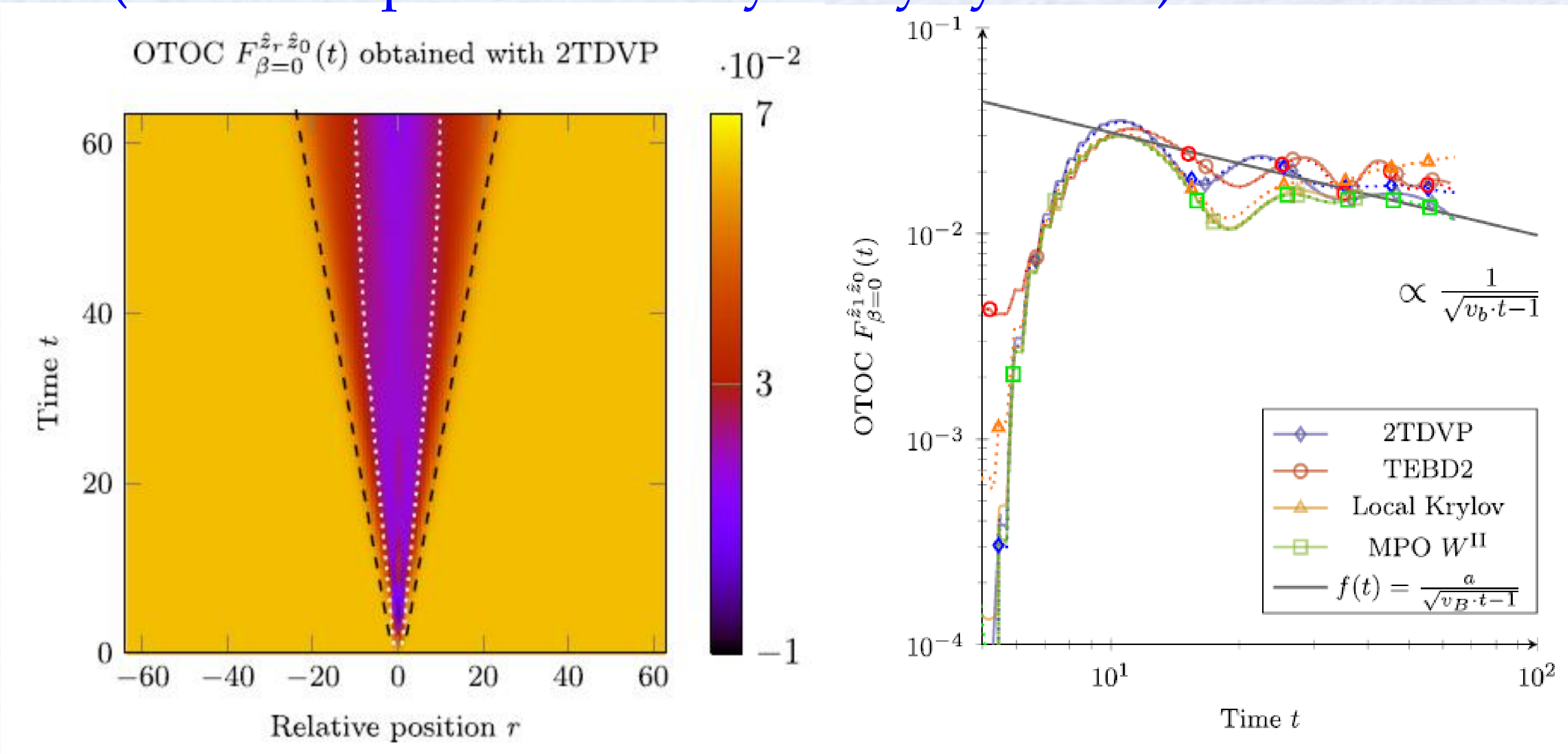
Quantum Quenches (simulate cold gases experiments)



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

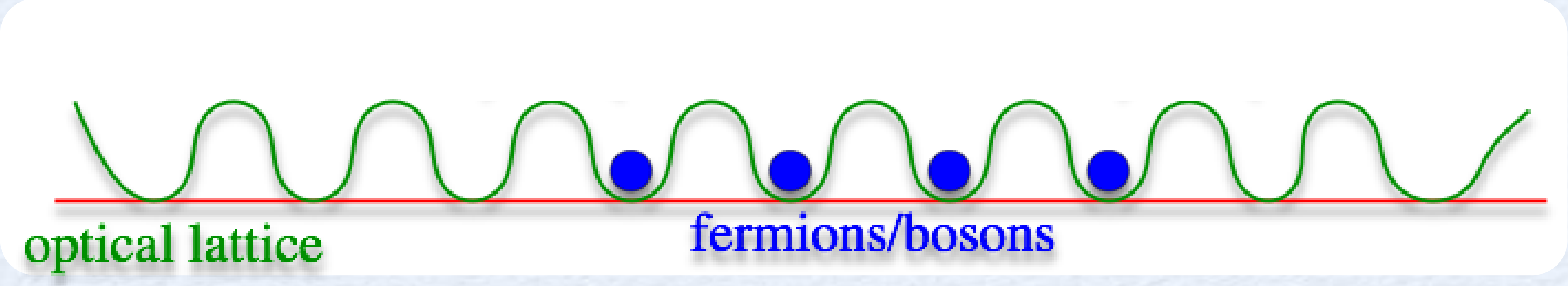


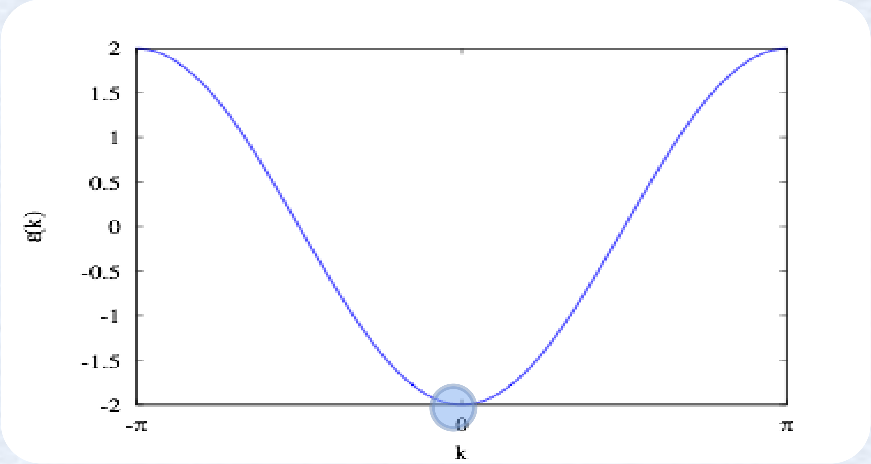
Out-of-time-order, OTOCs
(chaos in quantum many body systems)



Example 1:
Bloch Oscillations for interacting systems

Idea: tilt the lattice or apply a field and look at center of mass motion





➟ Constant force "drags" particle through Brillouin zone, Bragg scattering leads to change of direction:

$$\begin{aligned} \varepsilon(k) &= -2J\cos(k) && \text{dispersion relation 1D free fermions} \\ \dot{k} = E &\Rightarrow k(t) = k_0 + Et && E \text{ external field} \\ v_g(t) &= \frac{\partial \varepsilon[k(t)]}{\partial k} && \text{group velocity} \\ \Rightarrow x_{CM}(t) &\sim \frac{2J}{E}\cos(Et) && \text{center of mass motion} \end{aligned}$$

➟ Bloch oscillations for non-interacting systems

effect of interactions?

[Probe phase diagram: A.V. Gorshkov, S.R. Manmana et al., PRL (2011);
J. Carrasquilla, S.R. Manmana, M. Rigol PRA (2013)]

Example 1: Bloch Oscillations for interacting systems

[J. Carrasquilla, S.R. Manmana & M. Rigol, PRA **87**, 043606 (2013)]

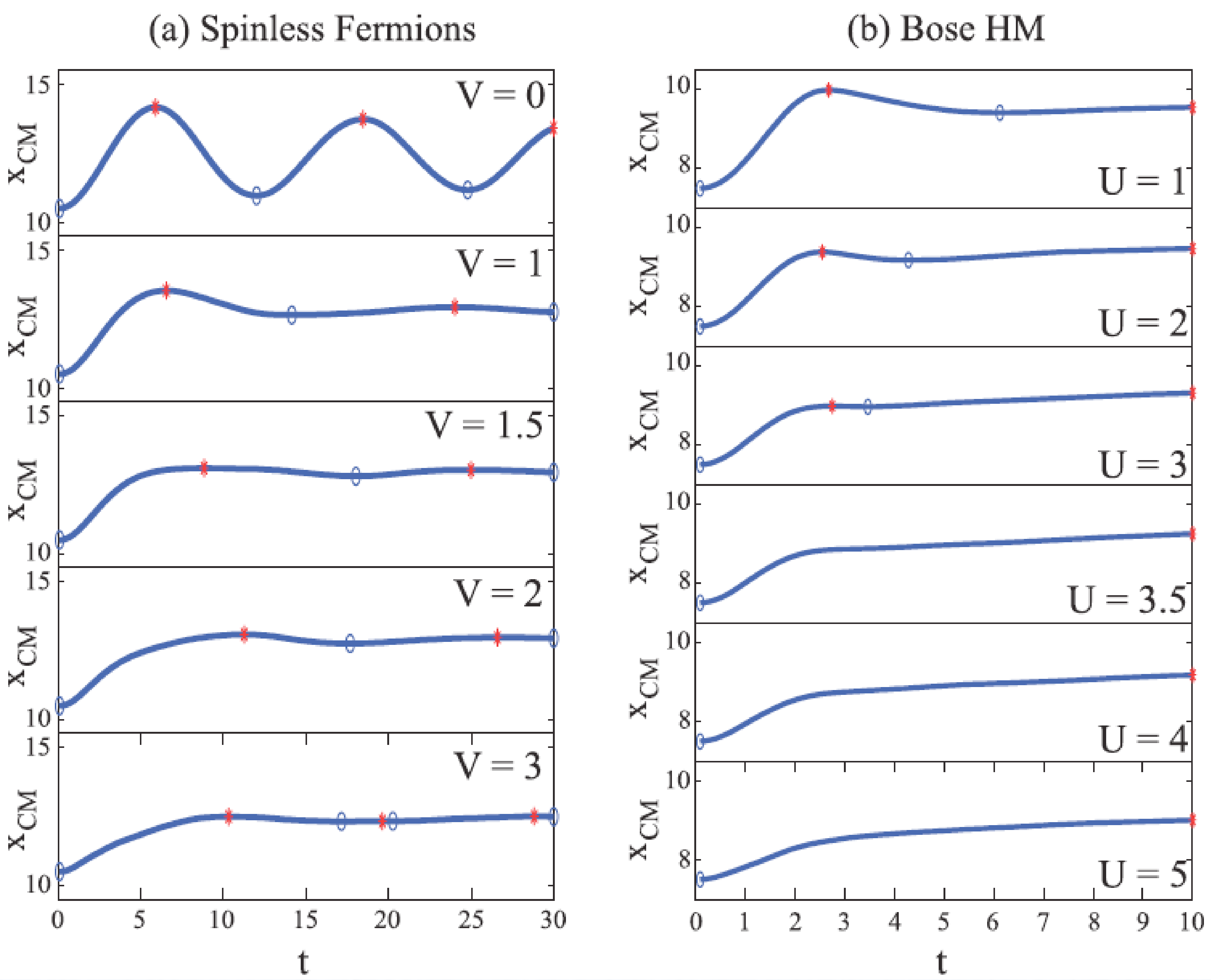
Spinless fermions at half filling:

$$H^{\mathrm{tV}} = -\sum_j t_j \left(c^\dagger_{j+1} c_j + c^\dagger_j c_{j+1}\right) + \sum_j V_j \, n_j n_{j+1}$$

Bose-Hubbard model at integer filling:

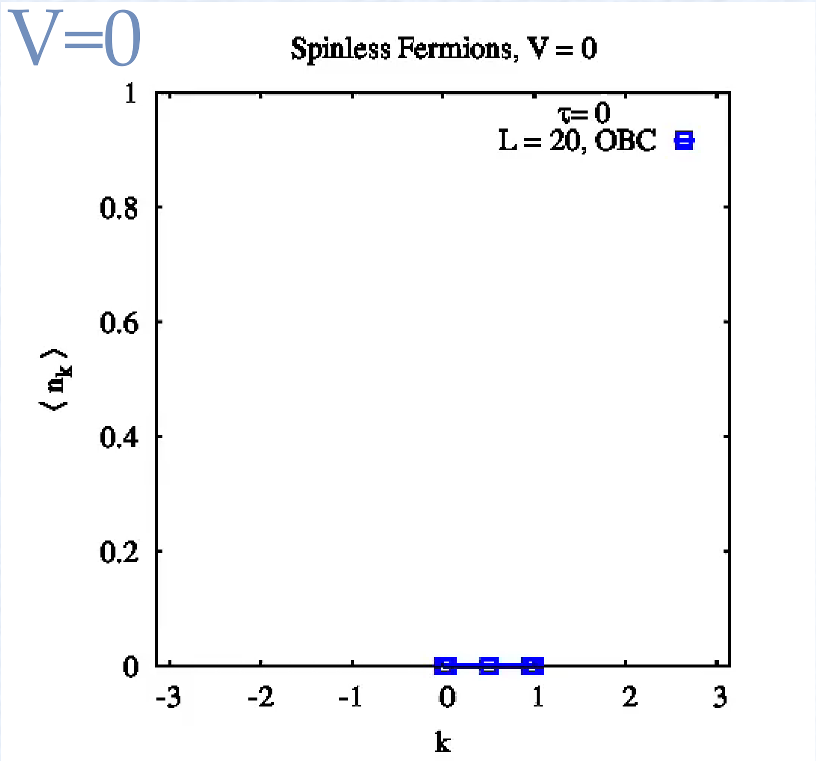
$$H^{\mathrm{BHM}} = -J \sum_{\langle i,j \rangle} \left(b^\dagger_i b_j + h.c.\right) + \frac{U}{2} \sum_i n_i (n_i - 1)$$

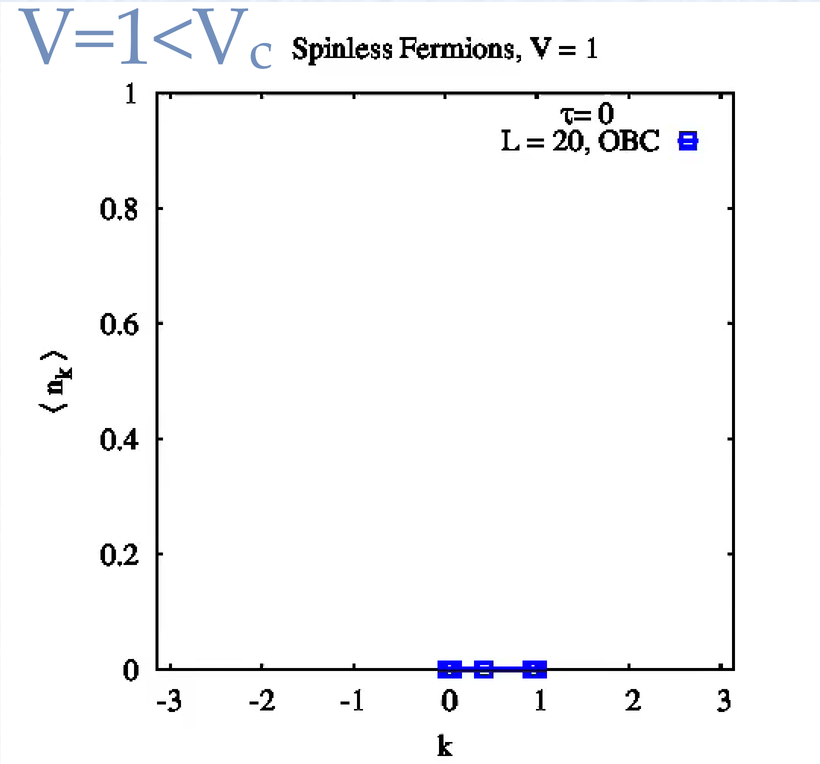
Center-of-Mass Motion:

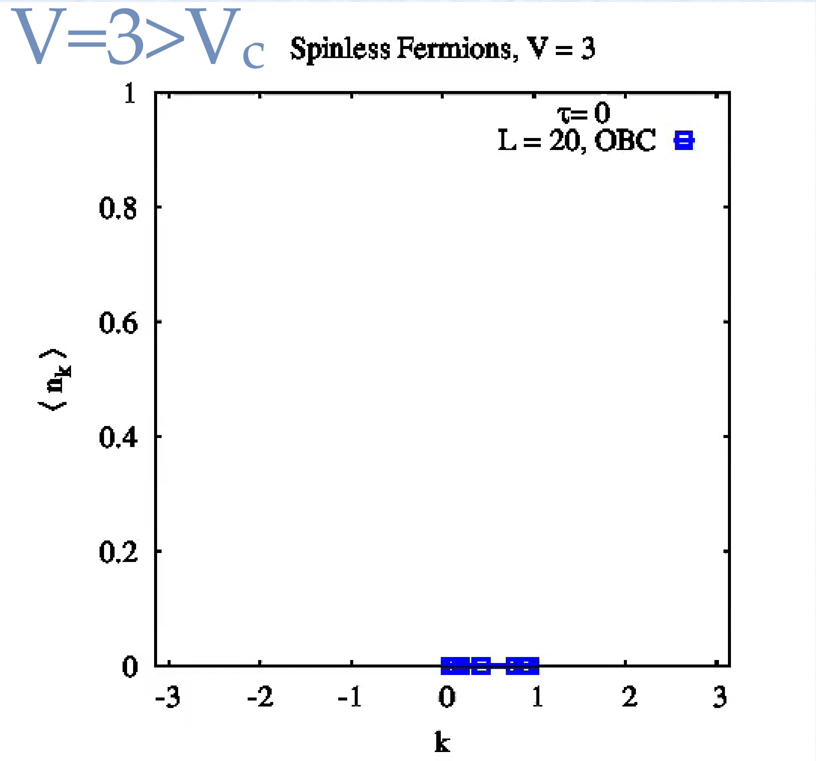


Example 1:
Bloch Oscillations for interacting systems

Time evolution of <n(k)>:







- Non-interacting systems: some dephasing, but no relaxation
- Interacting systems: “better” relaxation the stronger the interaction

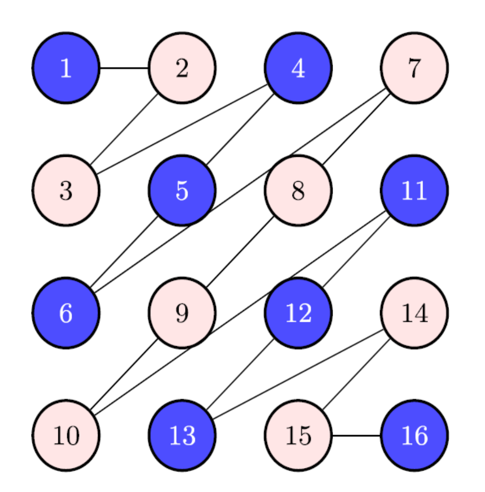
Open Questions:
Nature of (quasi-)stationary state? Effect of dissipation? Connect to condensed-matter systems?

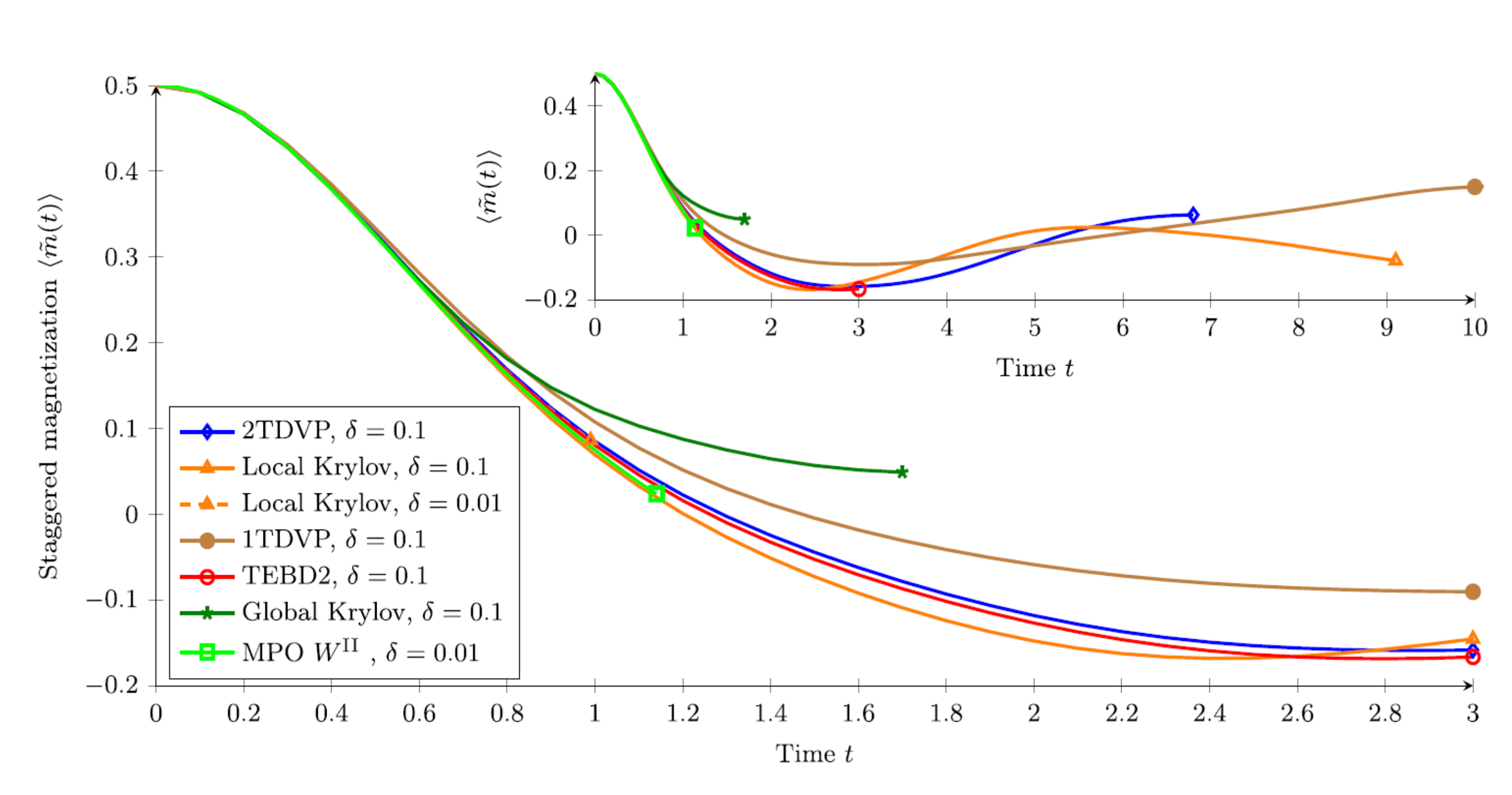
Today's Frontier: Time evolution in two dimensions?

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

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

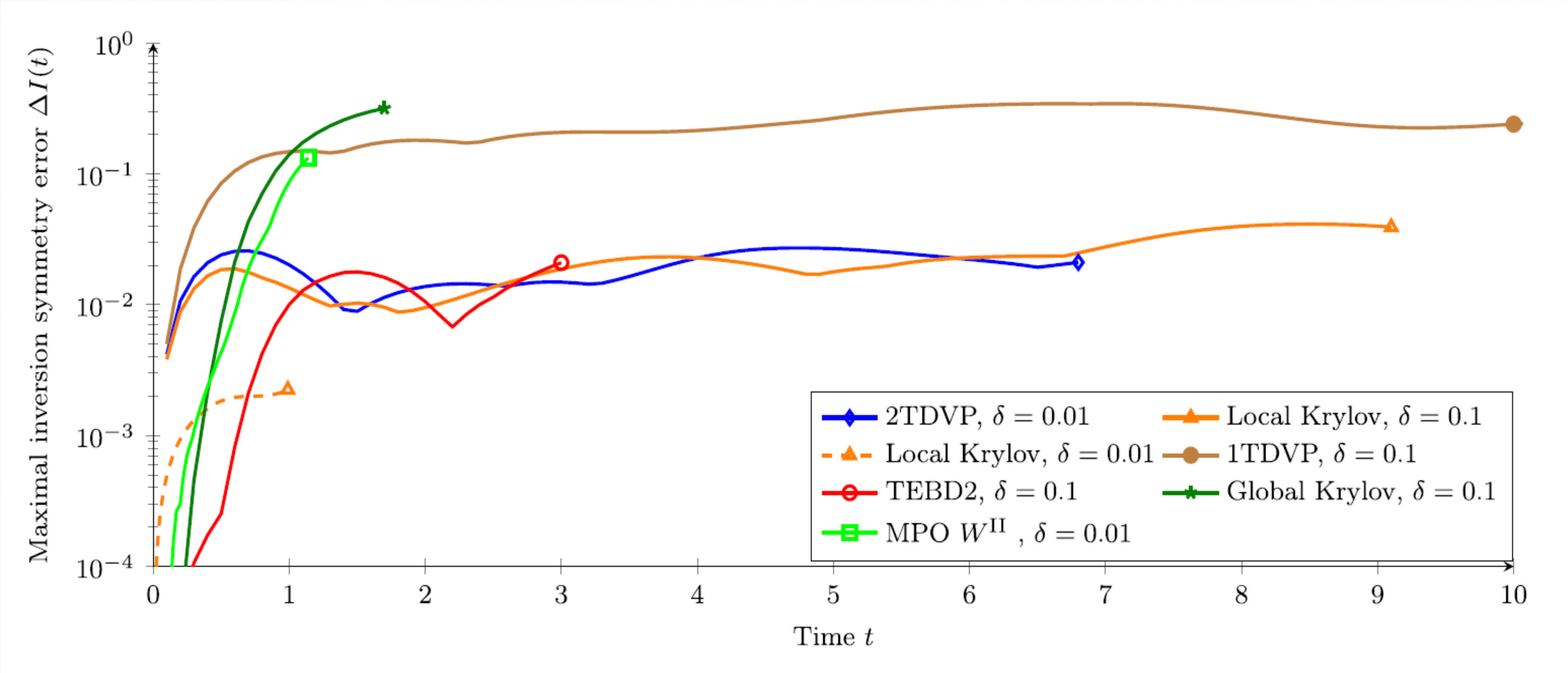
$$|\psi(0)\rangle = \bigotimes_{i\in A} |\downarrow\rangle_i \bigotimes_{j\in B} |\uparrow\rangle_j$$





Fixed bond-dimension m=200:

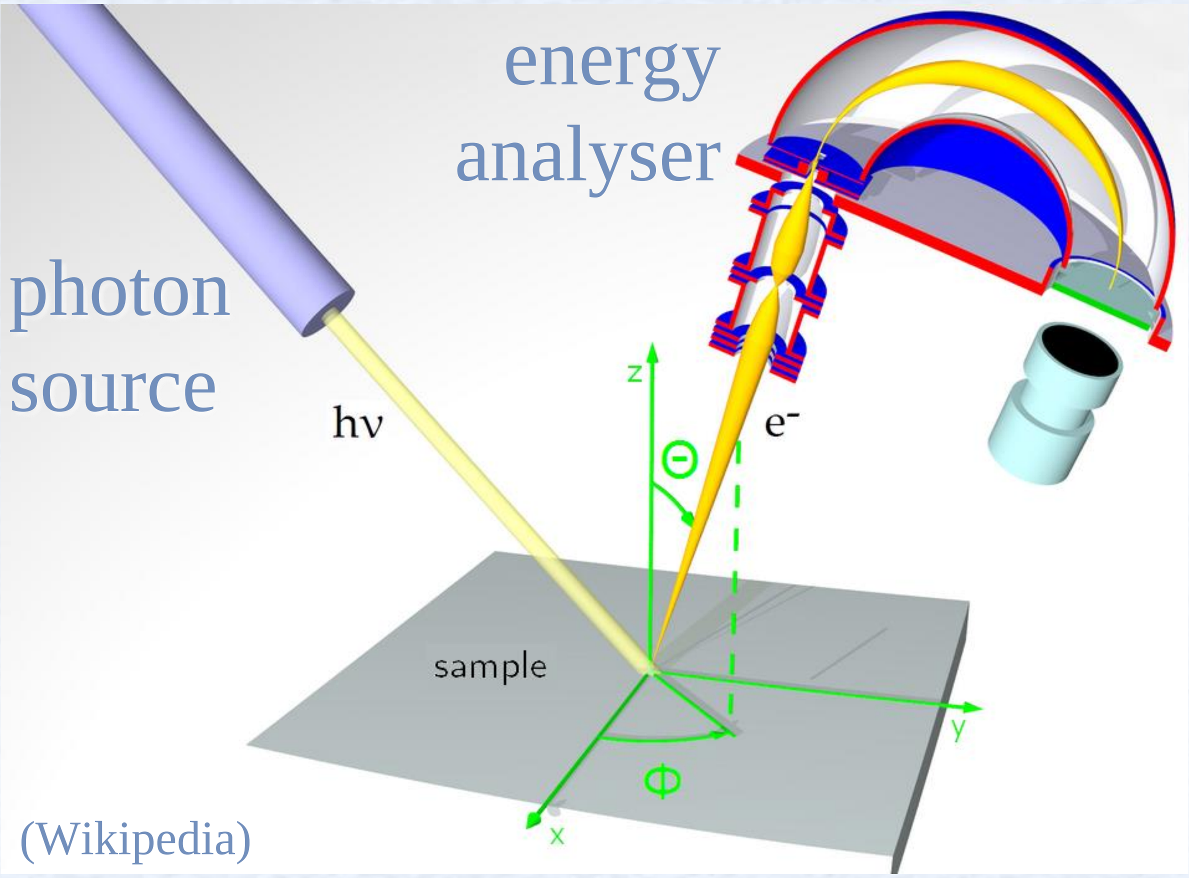
Errors grow rapidly, but some methods perform better than others at short times



Linear Response Dynamics at $T=0$

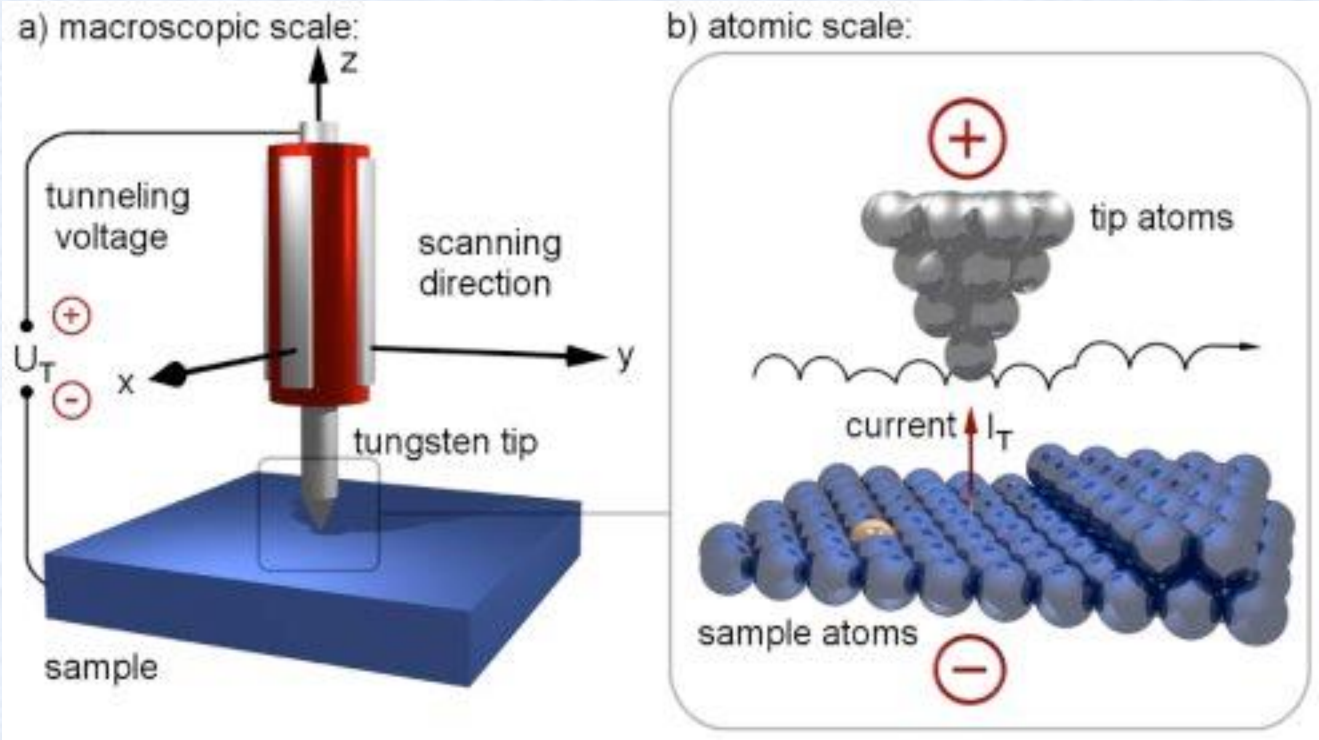
Characterize Many-Body Systems: Dynamical Spectral Functions

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: Dynamical correlation functions

- time-dependent perturbation

$$\mathcal{H}(t) = \mathcal{H}_0 - h_A \, \mathrm{e}^{i\,\omega\,t} \, A$$

- linear response:

$$\frac{\mathrm{d}}{\mathrm{d}h_A} \int\limits_{-\infty}^{\infty} \mathrm{d}t \, \langle B(t) \rangle \Bigg|_{h_A=0} = \int\limits_{-\infty}^{\infty} \mathrm{d}t \, \mathrm{e}^{i\,\omega\,t} \, \langle \mathcal{T} \, B(t) \, A \rangle_0 = \int\limits_{-\infty}^{\infty} \mathrm{d}t \, \sum_n \langle \Psi_0 | B | n \rangle \, \langle n | A | \Psi_0 \rangle \, \mathrm{e}^{i\,t\,(\omega - (E_n - E_0))}$$

$$= 2\pi \sum_n \langle \Psi_0 | B | n \rangle \, \langle n | A | \Psi_0 \rangle \, \delta(\omega - (E_n - E_0))$$

with

$$\mathcal{H}_0 \, | n \rangle = E_n \, | n \rangle$$

- express via Green's functions

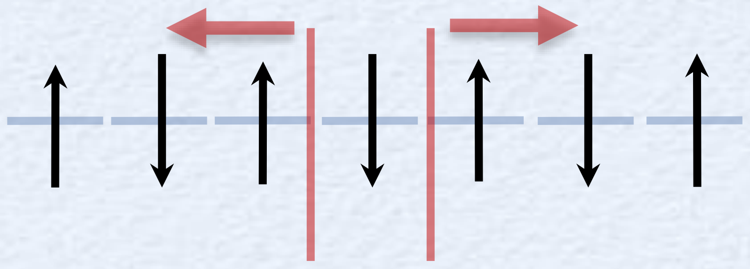
$$C_{A^\dagger, A}(\omega) = \mathrm{Im} G_A(\omega + i\,\eta + E_0) \,, \quad G_A(z) = \langle \Psi_0 | \, A^\dagger \, (z - \mathcal{H})^{-1} \, A \, | \Psi_0 \rangle$$

Linear Response: Spectral Functions at Finite Field

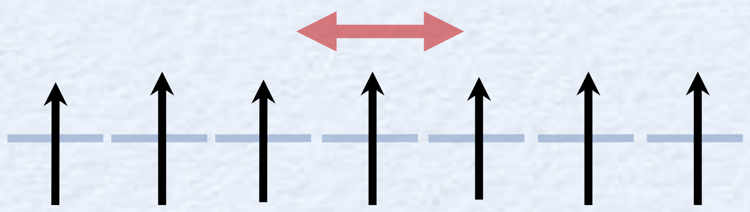
Dynamical structure factor $S^z(k,\omega)$ of a S-1/2 Heisenberg chain when changing an external magnetic field:

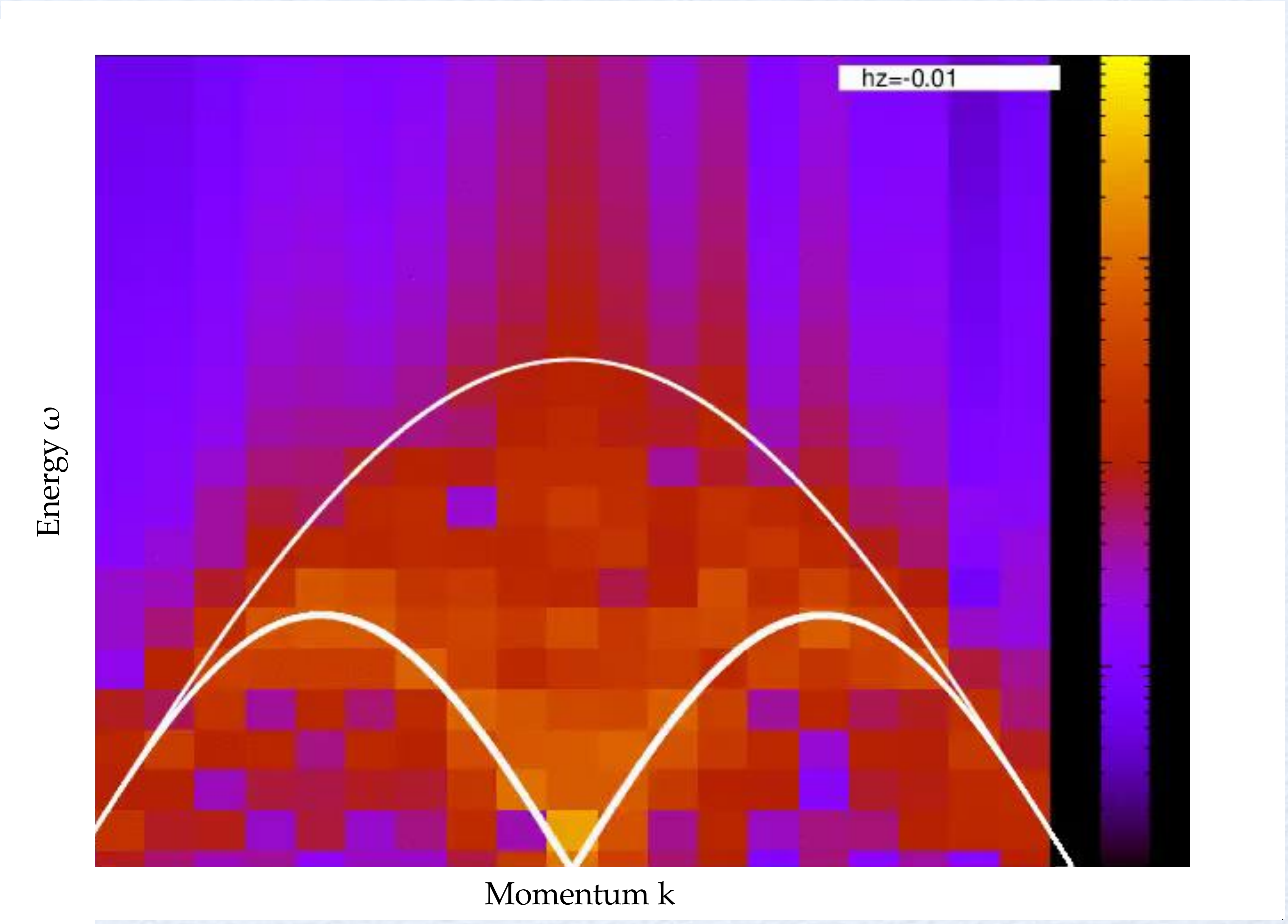
$$\mathcal{H} = J\sum_i \vec{S}_i \cdot \vec{S}_{i+1} - B\sum_i S_i^z$$

small B: spinons



large B: magnons





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).

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

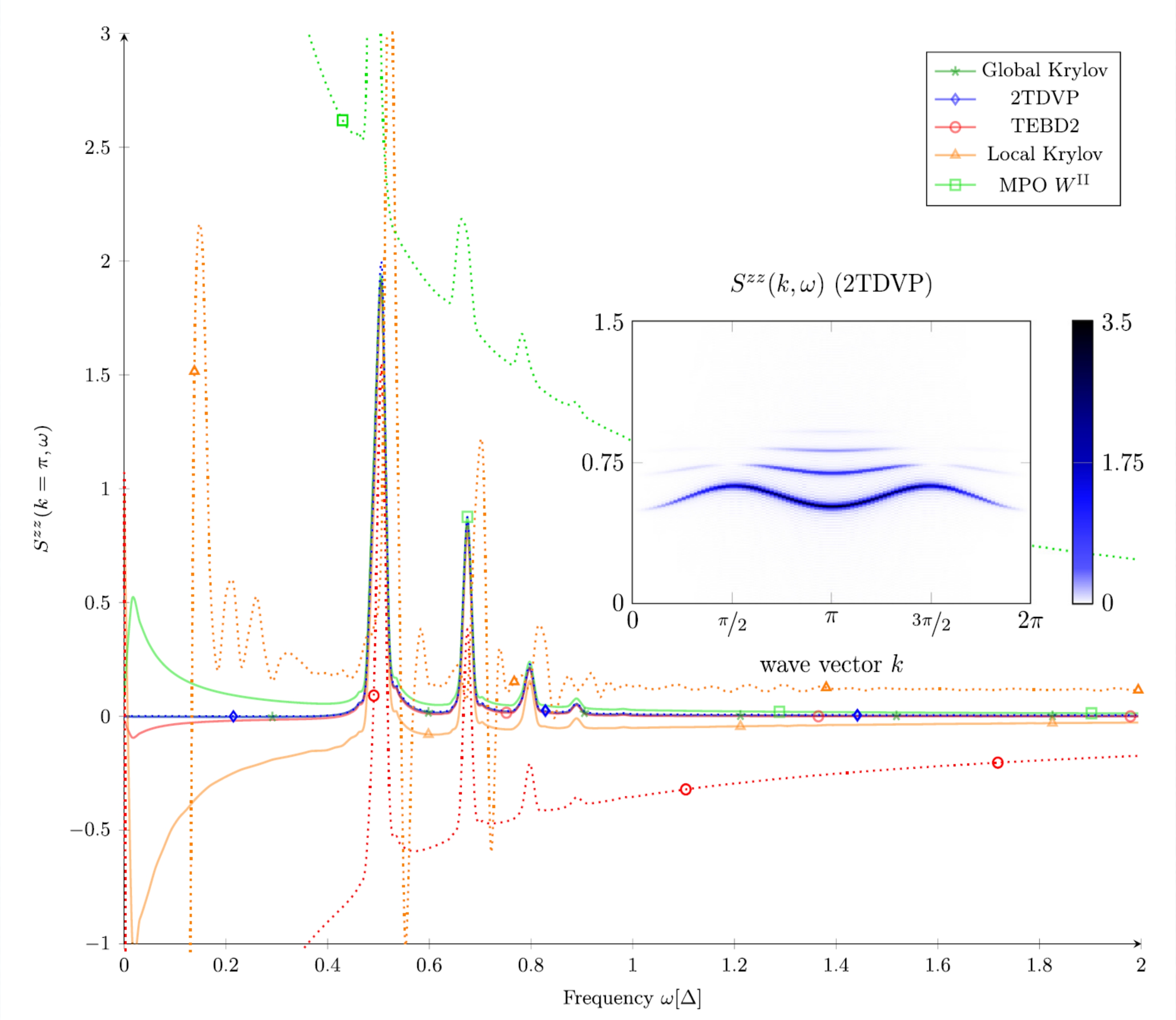
Dynamical correlation functions: Approach using real-time evolution

$$\hat{H} = J\sum_{j=1}^{L}\left[\hat{s}^x_j\hat{s}^x_{j+1} + \hat{s}^y_j\hat{s}^y_{j+1} + \Delta\hat{s}^z_j\hat{s}^z_{j+1} - h^s_j\hat{s}^z_j\right]$$

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

$$S^{zz}(q,\omega) = \frac{1}{L}\sum_{j=1}^{L} e^{-iq(j-L/2)}\int_{-\infty}^{\infty} dt\; e^{i\omega t}\langle\hat{s}^z_j(t)\hat{s}^z_{L/2}(0)\rangle_{cc}$$

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



Some methods show artifacts at low frequencies – not TDVP

Salvatore R. Manmana

Linear Response Dynamics at $T>0$

Dynamical correlation functions: $T = 0$ vs. $T > 0$

Dynamical correlation functions at T = 0:

$$G_A(\omega) = -\frac{1}{\pi}\mathrm{Im}\left\langle \psi_0 \left| A^\dagger \frac{1}{\omega + E_0 + i\varepsilon - H} A \right| \psi_0 \right\rangle = \sum_n \left| \langle n | A | \psi_0 \rangle \right|^2 \delta\left(\omega - (E_n - E_0)\right)$$

$$\mathcal{H}_0 \left| n \right\rangle = E_n \left| n \right\rangle$$

Dynamical correlation functions at T > 0:

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

➟ Need the full spectrum...difficult ☹

Ways out: continued fraction expansion, (D)DMRG, QMC,...
Here: DMRG + Chebyshev expansions

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

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† 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"

Dynamical correlation functions: Lanczos recursion

[E. Dagotto, RMP (1994)]

☞ use continued fraction expansion (CFE)

$$G_A(z) = -\frac{1}{\pi}\mathrm{Im}\left\langle \psi_0 \left| A^\dagger \frac{1}{z-\mathcal{L}} A \right| \psi_0 \right\rangle = -\frac{1}{\pi}\mathrm{Im}\frac{\langle \Psi_0 | A^\dagger A | \Psi_0 \rangle}{z - a_0 - \frac{b_1^2}{z - a_1 - \frac{b_2^2}{z - ..}}}$$

via Lanczos recursion

$$|f_0\rangle = A|\Psi_0\rangle, \qquad |f_{n+1}\rangle = \mathcal{L}|f_n\rangle - a_n|f_n\rangle - b_n^2|f_{n-1}\rangle$$

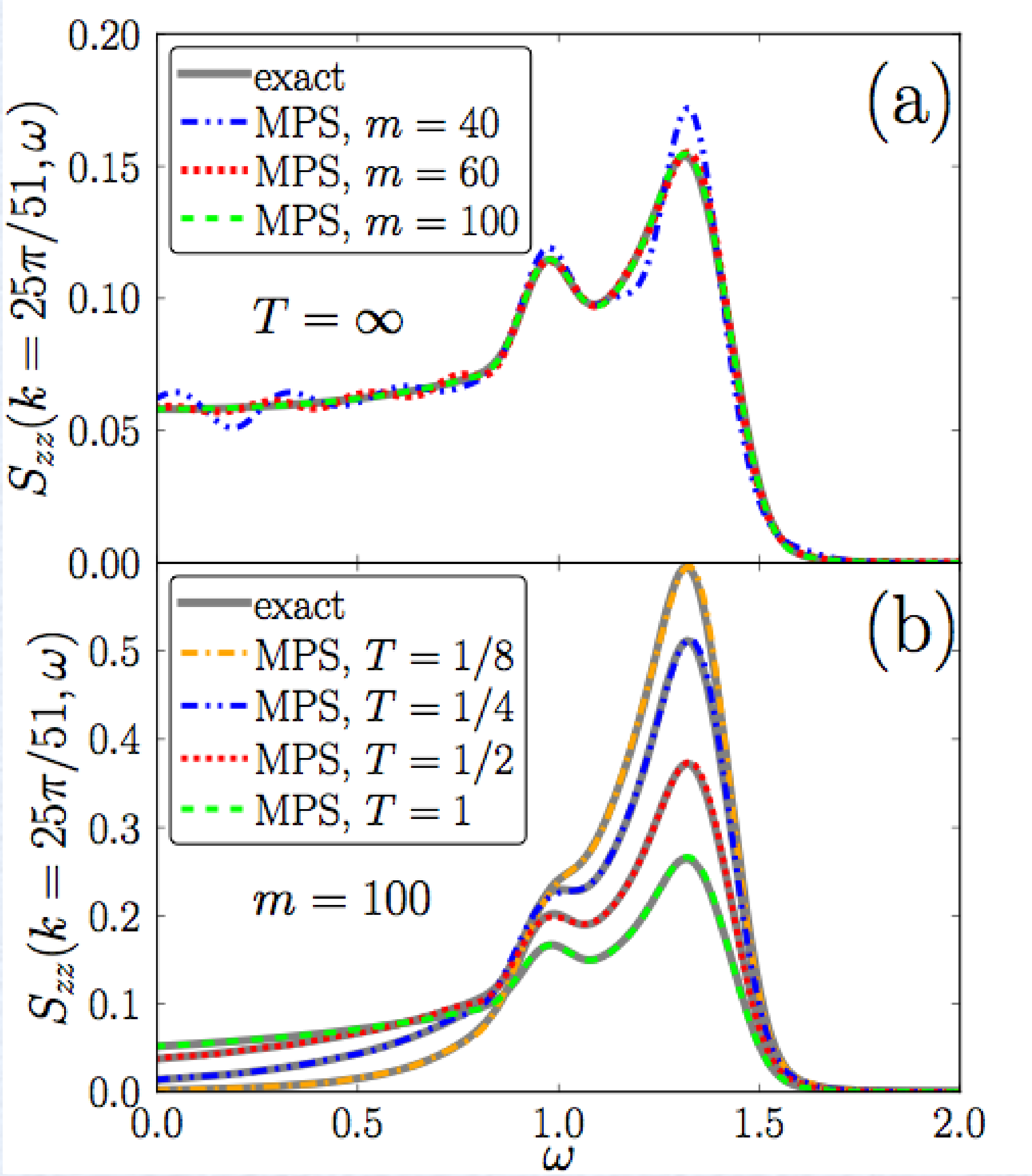
$$a_n = \frac{\langle f_n|\mathcal{L}|f_n\rangle}{\langle f_n|f_n\rangle}, \qquad b_{n+1}^2 = \frac{\langle f_{n+1}|f_{n+1}\rangle}{\langle f_n|f_n\rangle}, \qquad b_0 = 0$$

Liouvillian finite-T approach: comparison to exact results

$$H_{XX} = J \sum_{i}^{L-1} \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right)$$

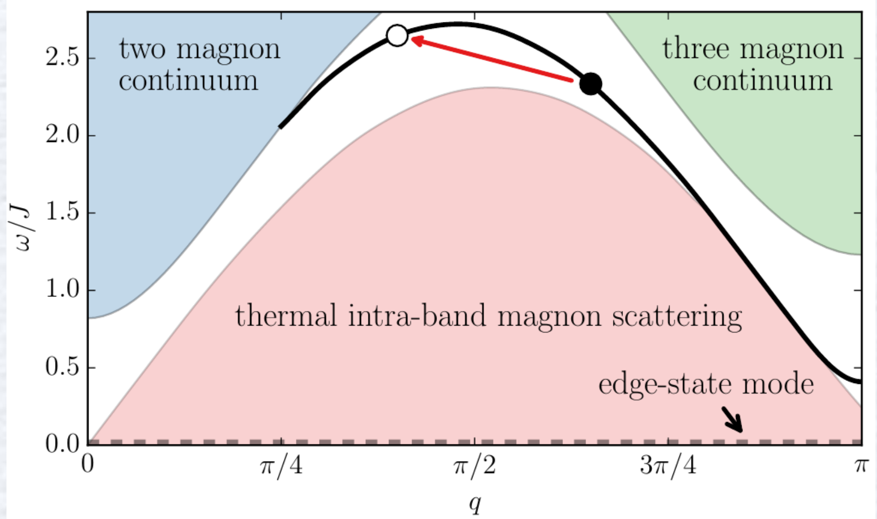
[A. Tiegel, et al., PRB (R, 2014)]

$$S_k^\alpha = \sqrt{\frac{2}{L+1}} \sum_{i=1}^{L} \sin(ki)\, S_i^\alpha$$



Excellent agreement with exact results!

Finite-T dynamics in spin-1 chains



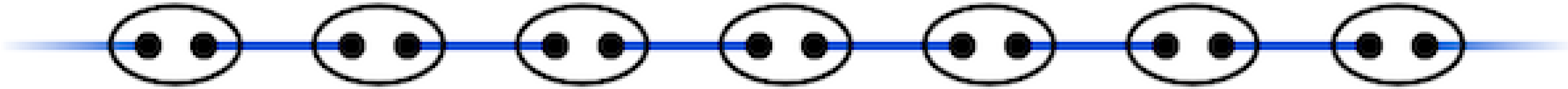
➠ New features in the spectra at T>0?

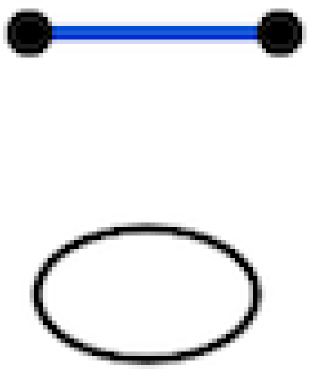
Spin-1 chains:

AKLT state

Nobel Prize
2016

Sketch of the AKLT state:



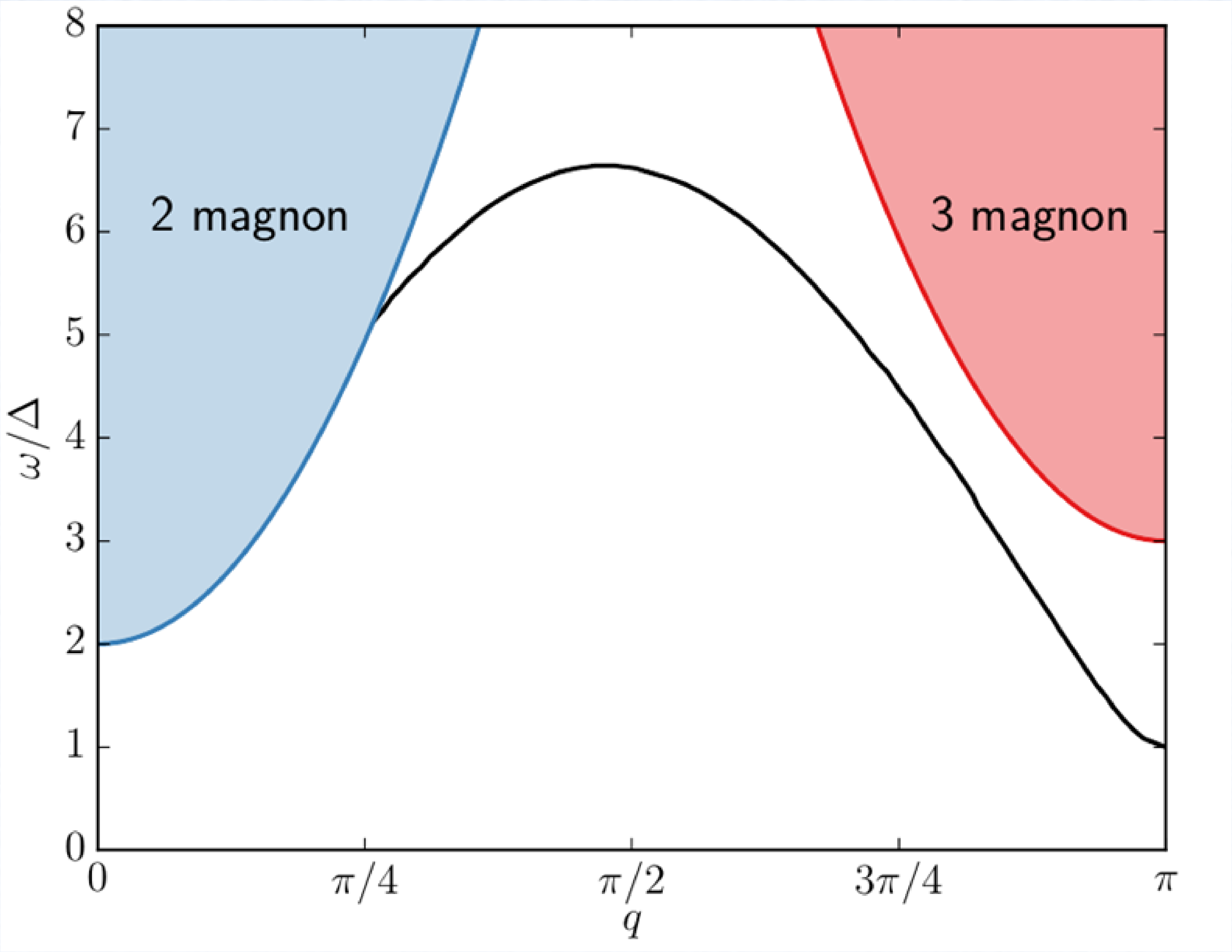


$$= \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)$$

$$= |+\rangle\langle\uparrow\uparrow| + |0\rangle \frac{\langle\uparrow\downarrow| + \langle\downarrow\uparrow|}{\sqrt{2}} + |-\rangle\langle\downarrow\downarrow|$$

- „Topological“ phase (symmetry protected topol. state, SPT)
- Exact ground state of $\hat{H} = \sum_i \left[\vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3} \left(\vec{S}_i \cdot \vec{S}_{i+1} \right)^2 \right]$
- No local order parameter, but string order parameter
- Fractional excitations: effective S=1/2 at the edges

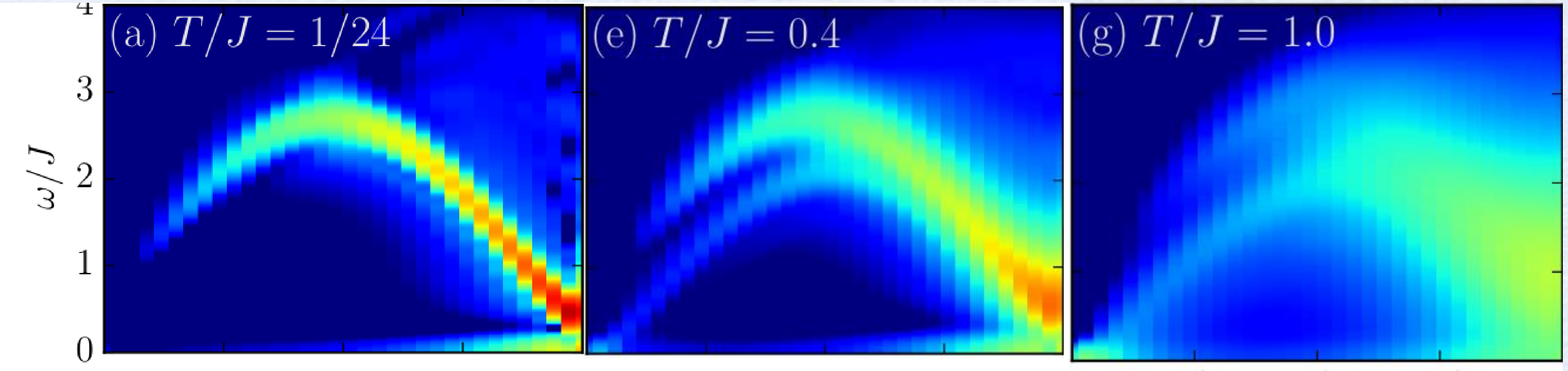
Spin-1 chains: Spectral functions at T=0



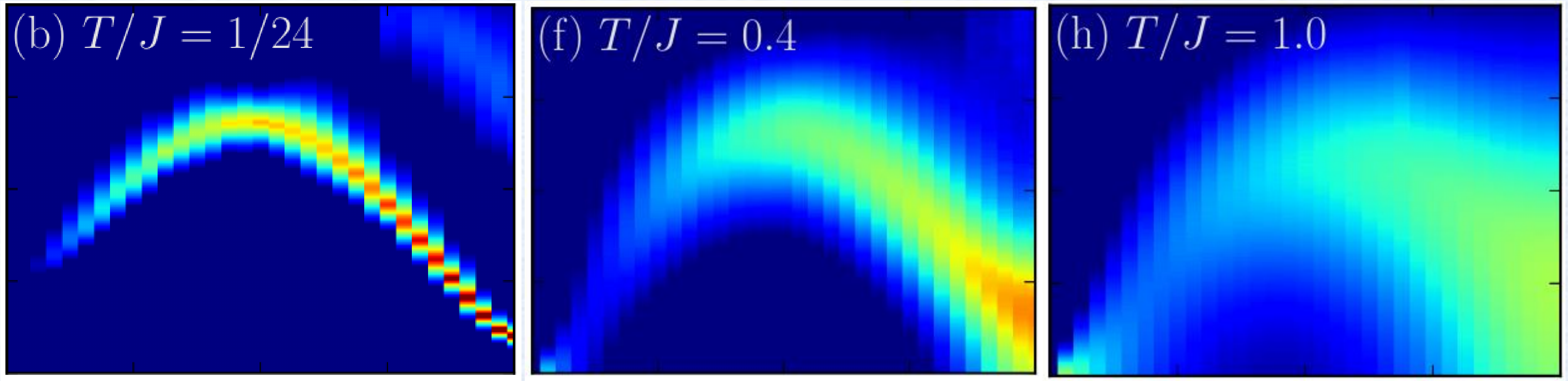
S.R. White & I. Affleck, PRB (2008)

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

DMRG, OBC, L=32:



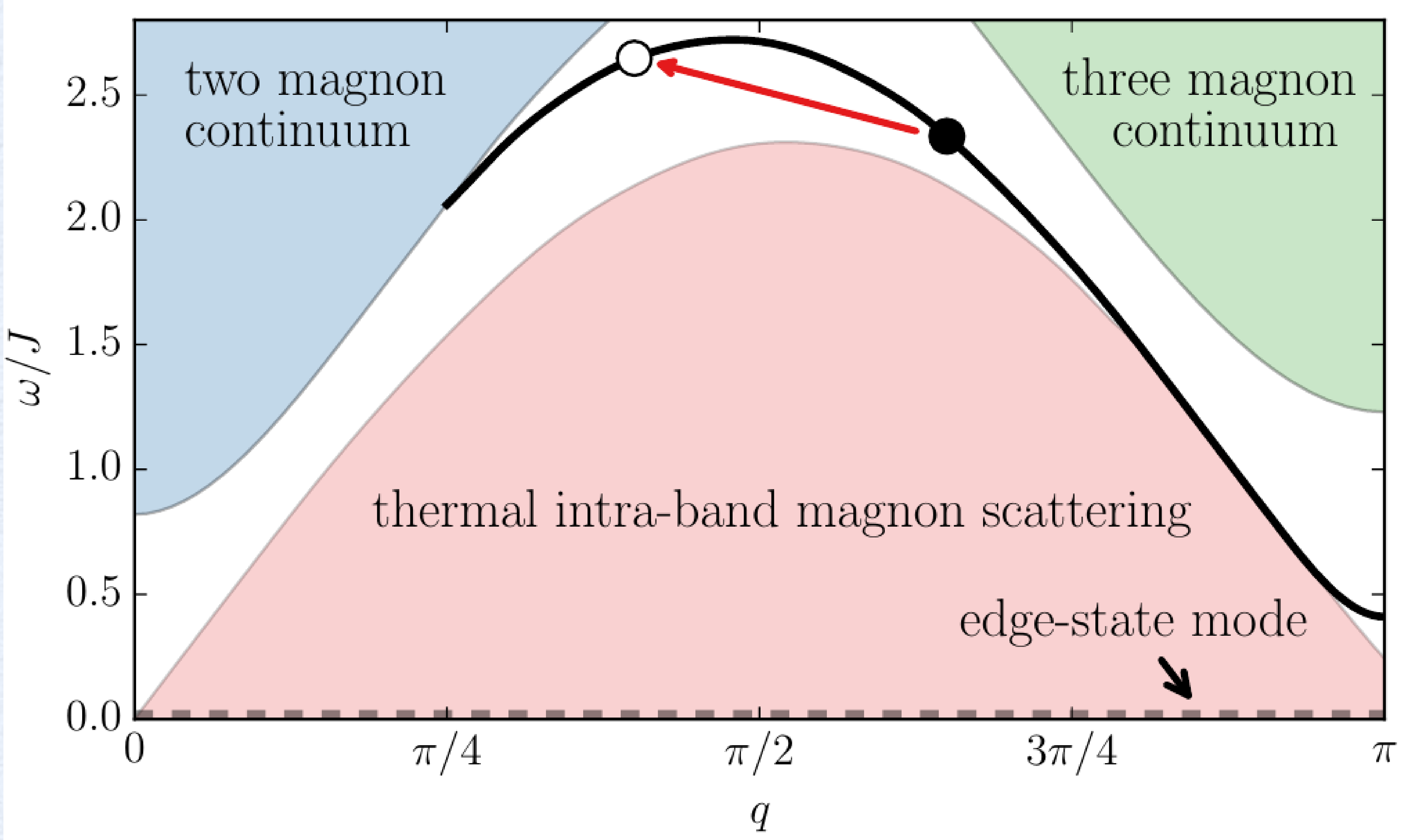
QMC, PBC, L=64:



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

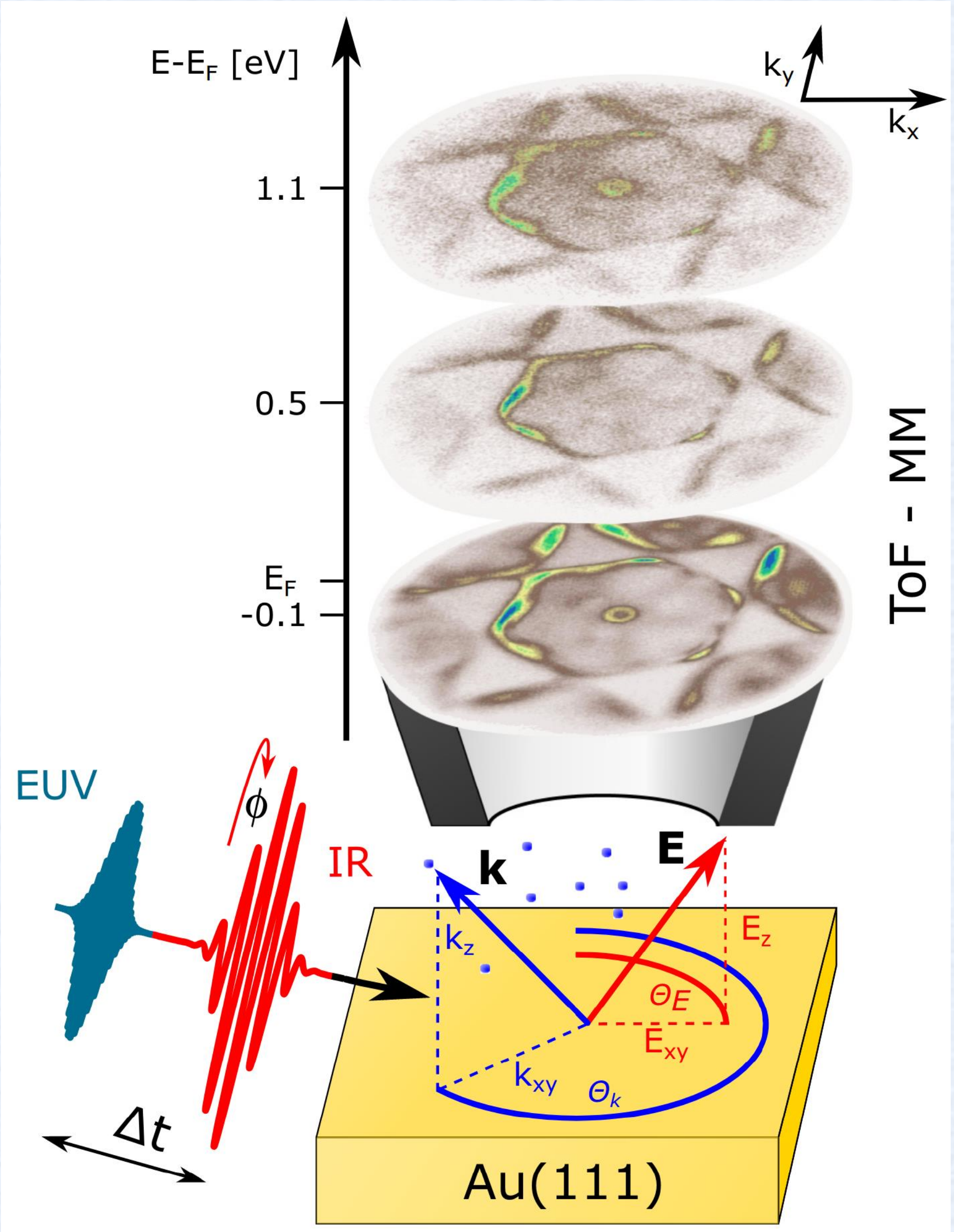


J. Becker, T. Köhler, A.C. Tiegel, S.R. Manmana, S. Wessel, and A. Honecker, PRB **96**, 060403(R) (2017).

Linear Response Dynamics Out-of-Equilibrium

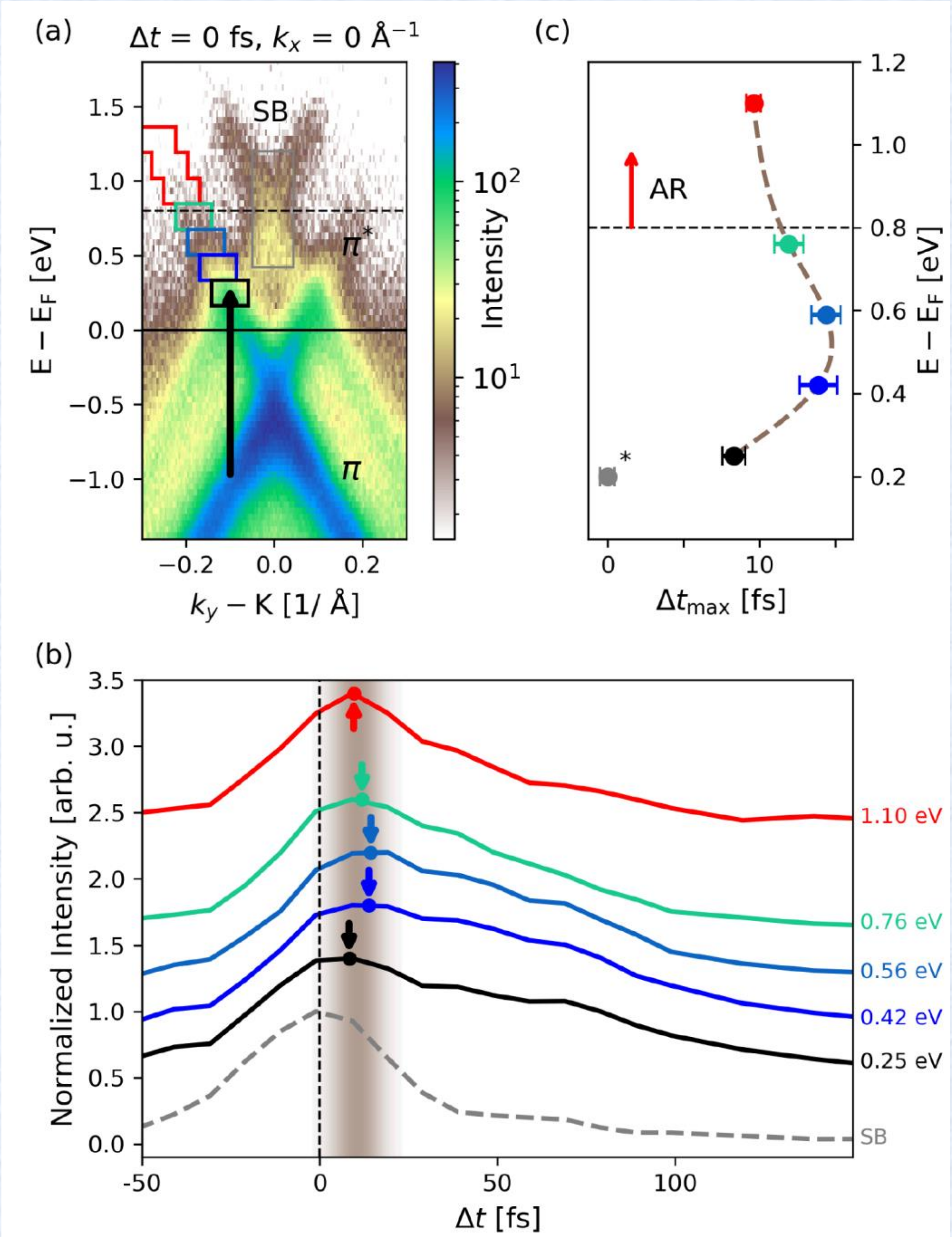
Excitation and Recombination: Time-resolved ARPES

New developments, e.g., „Momentum Microscope“



Observe Floquet states?

Time-resolved recombination processes?

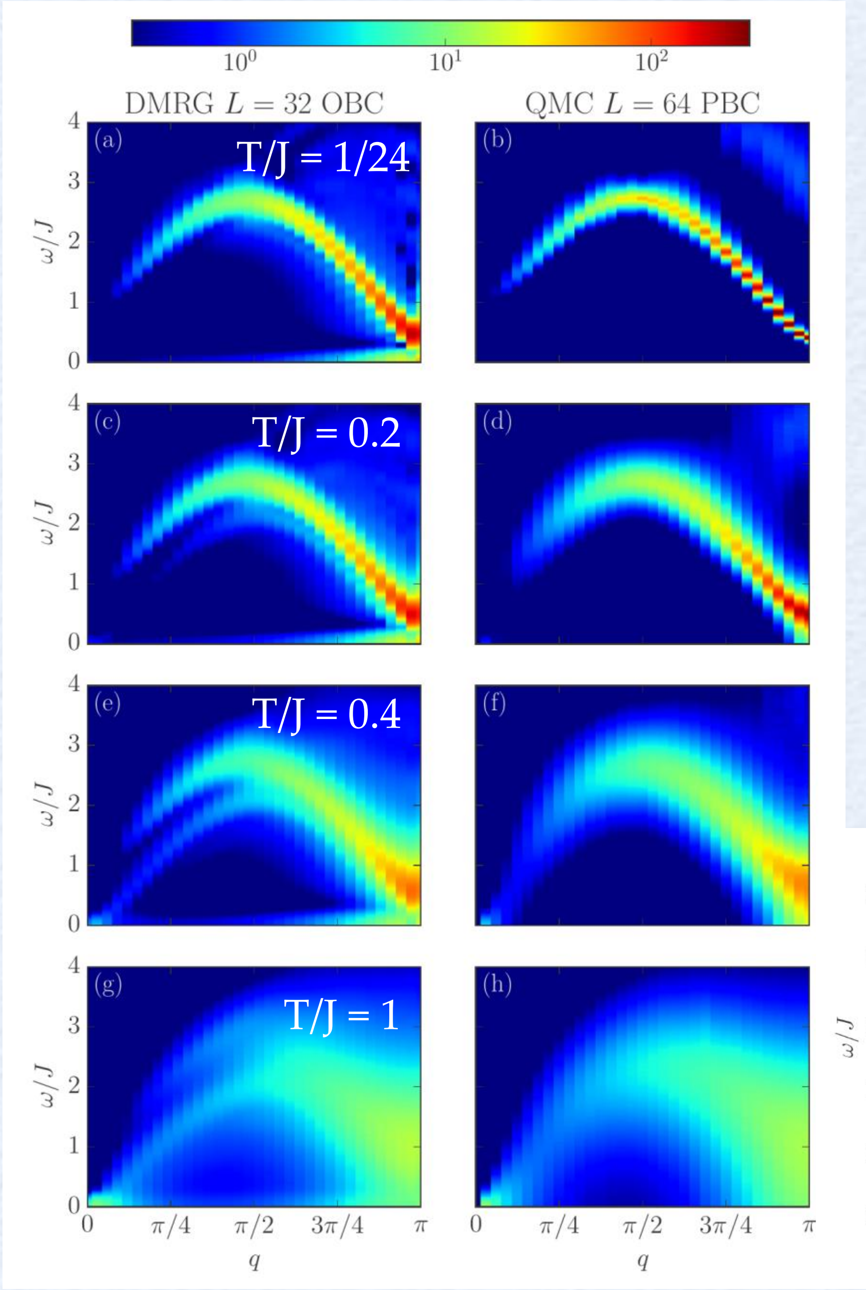


Electromagnetic dressing of the electron energy spectrum of Au(111) at high momenta, M. Keunecke et al., PRB (rapid comm.) **102**, 161403 (2020)

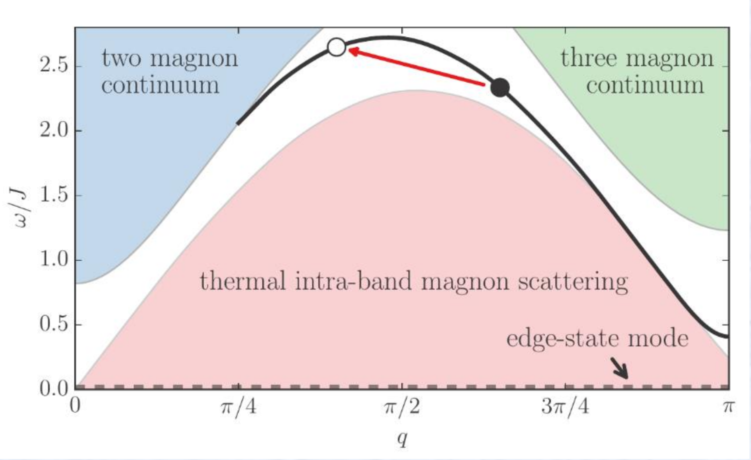
Direct Access to Auger Recombination in Graphene, M. Keunecke et al., arXiv:2012.01256

Thermal and Photoexcitations: Effect on Dynamical Properties

Heat up a spin-1 Heisenberg chain:

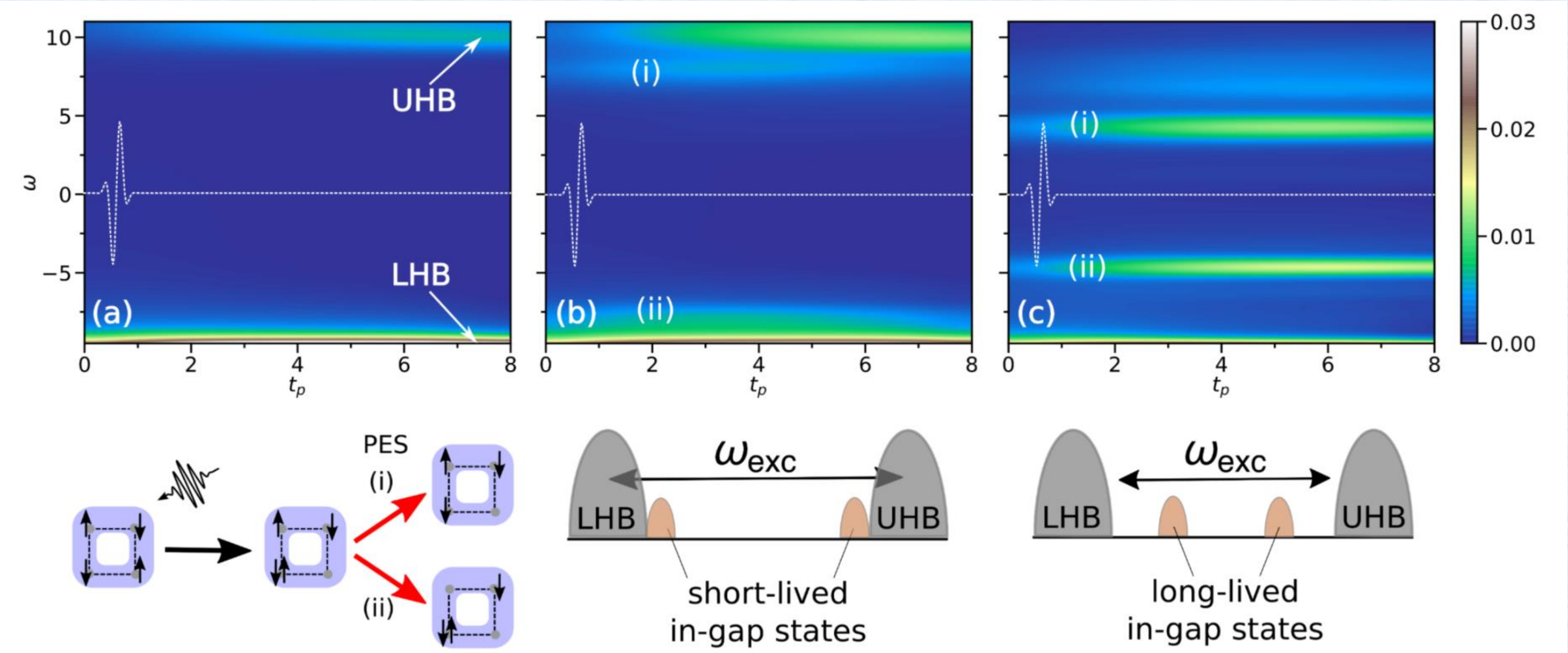


Reason for the new branch: magnon scattering



Finite-Temperature Dynamics and Thermal Intraband Magnon Scattering in Haldane Spin-One Chains, J. Becker et al., PRB (rapid comm.) **96**, 060403 (2017)

Excite a Hubbard-system with ultrashort laser pulses:



$$\hat{H} = -\sum_{\langle r,s\rangle,\sigma}\left(t_{\mathrm{h}}(t)\,\hat{c}^{\dagger}_{\sigma,r}\hat{c}_{\sigma,s} + \mathrm{h.c.}\right) - \mu\sum_r \hat{n}_r + U\sum_r \hat{n}_{\uparrow,r}\hat{n}_{\downarrow,r} + V\sum_{\langle r,s\rangle}\hat{n}_r\hat{n}_s$$

$U = 25, V = 0, 3, 6$ (2D model)

Reason/interpretation of in-gap states: formation of excitons (due to n.n. interaction)

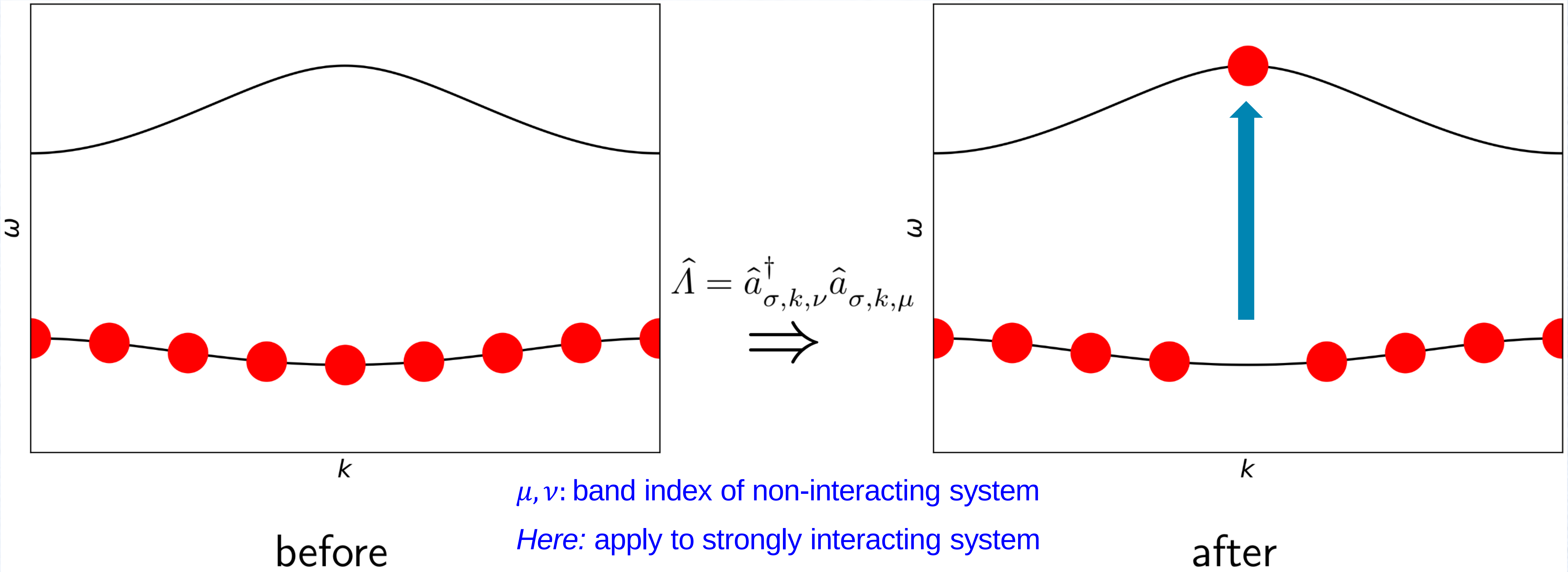
Photo-enhanced excitonic correlations in a Mott insulator with nonlocal interactions, N. Bittner et al., PRB **101**, 085127 (2020)

- Other in-gap states / new branches in nonequilibrium systems? Quasiparticles?
- Relation between thermal and noneq.-excitations?

Spin-selective excitations: Electron-hole excitation & band structure

Constantin Meyer and SRM, in preparation

Modeling of an electron-hole excitation in a correlated system:



- Non-interacting systems: well defined – but excited state is an eigenstate, no relaxation
- Interacting systems: „bands“? Scattering will influence the effect of the excitation
- Need to consider time-dependent spectral functions
- Here: systematic study of a spin-selective electron-hole excitation in a Hubbard-system with separate bands

Electron-hole excitation: Time-dependent spectral fct. & band structure

- Expression in equilibrium and key property

$$\mathscr{A}_\sigma^<(k,\omega) = \mathscr{F}(\omega;t')\Big[\langle\Psi|\,\hat{a}^\dagger_{\sigma,k}(t')\,\hat{a}_{\sigma,k}\,|\Psi\rangle\Big] \propto \delta(\omega - \varepsilon_\sigma^<(k))$$

- Extension to time-dependent spectral function
  - Definition via Fourier transform over one time of a two-time Green's function

$$\mathscr{A}_\sigma^<(k,t',t) = \langle\Psi(t)|\,\hat{a}^\dagger_{\sigma,k}(t')\,\hat{a}_{\sigma,k}\,|\Psi(t)\rangle$$

  - $|\Psi(t)\rangle$: Time evolved state after excitation, quantum quench, pump pulse, ...
  - Here:

$$|\Psi(t=0)\rangle = \hat{\Lambda}\,|\mathrm{GS}\rangle$$

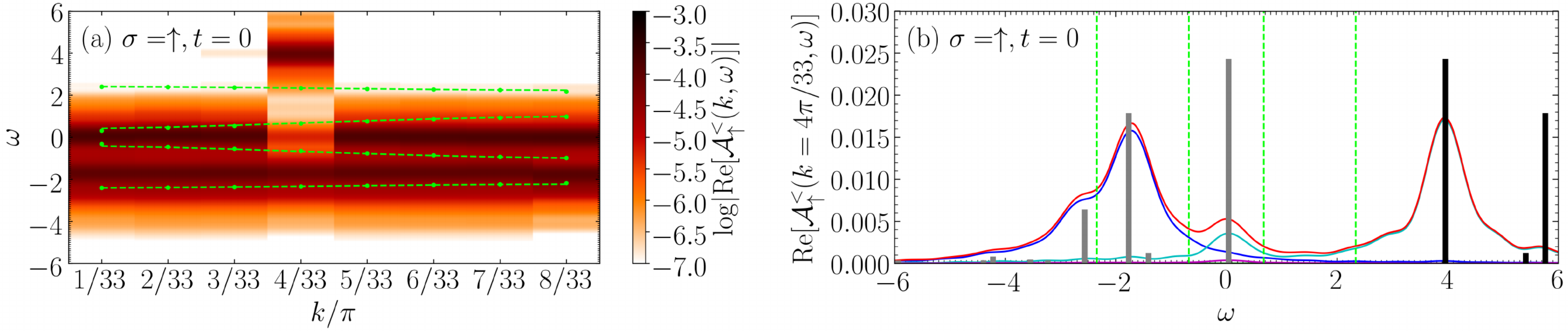
    for any excitation $\hat{\Lambda}$, e.g. photon absorption through electron-hole excitation
  - Transform to ω-space with artificial broadening η

$$\mathscr{A}_\sigma^<(k,\omega,t) = 2\mathrm{Re}\Big[\int_0^\infty \mathrm{d}t'\mathrm{e}^{-\mathrm{i}\omega t'}\mathrm{e}^{-\eta t'}\mathscr{A}_\sigma^<(k,t',t)\Big]$$

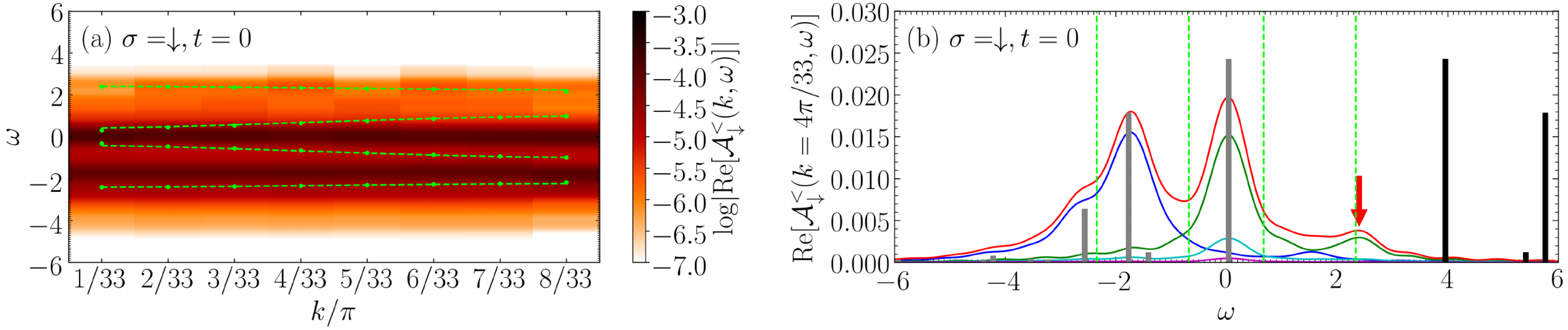
Electron-hole excitation: „shadow-band“ formation

C. Meyer & S.R. Manmana, arXiv:2109.07037

Electron-hole Excitation $\hat{\Lambda} = \hat{a}^{\dagger}_{\uparrow,k,\mu}\hat{a}_{\uparrow,k,\nu}$ $(U = 4,\ \Delta = 2)$



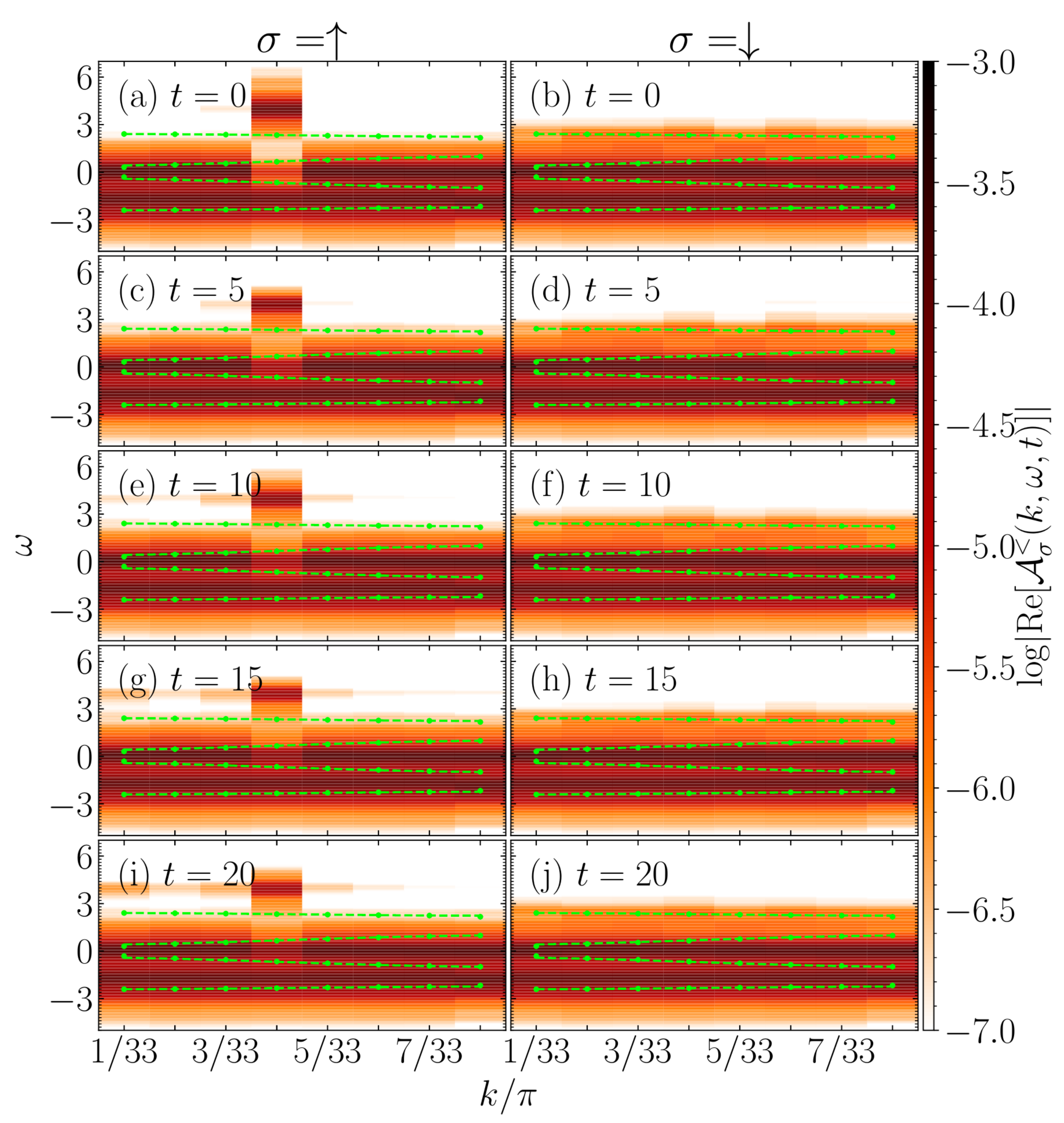
- Approximate modeling of spin-selective electron-hole excitation



- New in-gap feature in opposite spin direction

Electron-hole excitation: Stability of the „shadow-band“

C. Meyer & S.R. Manmana, arXiv:2109.07037



Electron-hole Excitation $\hat{\Lambda} = \hat{a}^{\dagger}_{\uparrow,k,\mu}\hat{a}_{\uparrow,k,\nu}$ $(U = 4,\ \Delta = 2)$

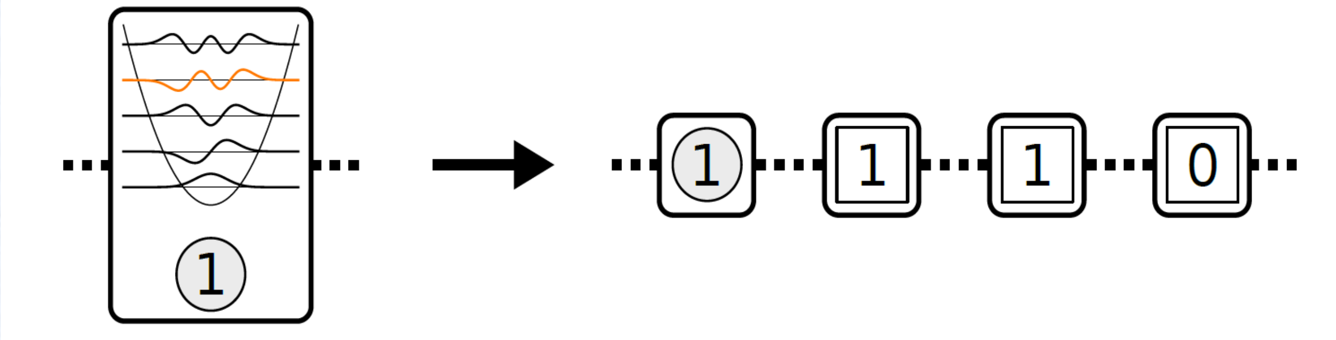
- Scattering within bands
- $\uparrow$: Redistribution over entire band
- $\downarrow$: Stable total weight over time

Further Developments:
Phonons, reduce entanglement

Purification: quantum numbers for systems without conserved quantities

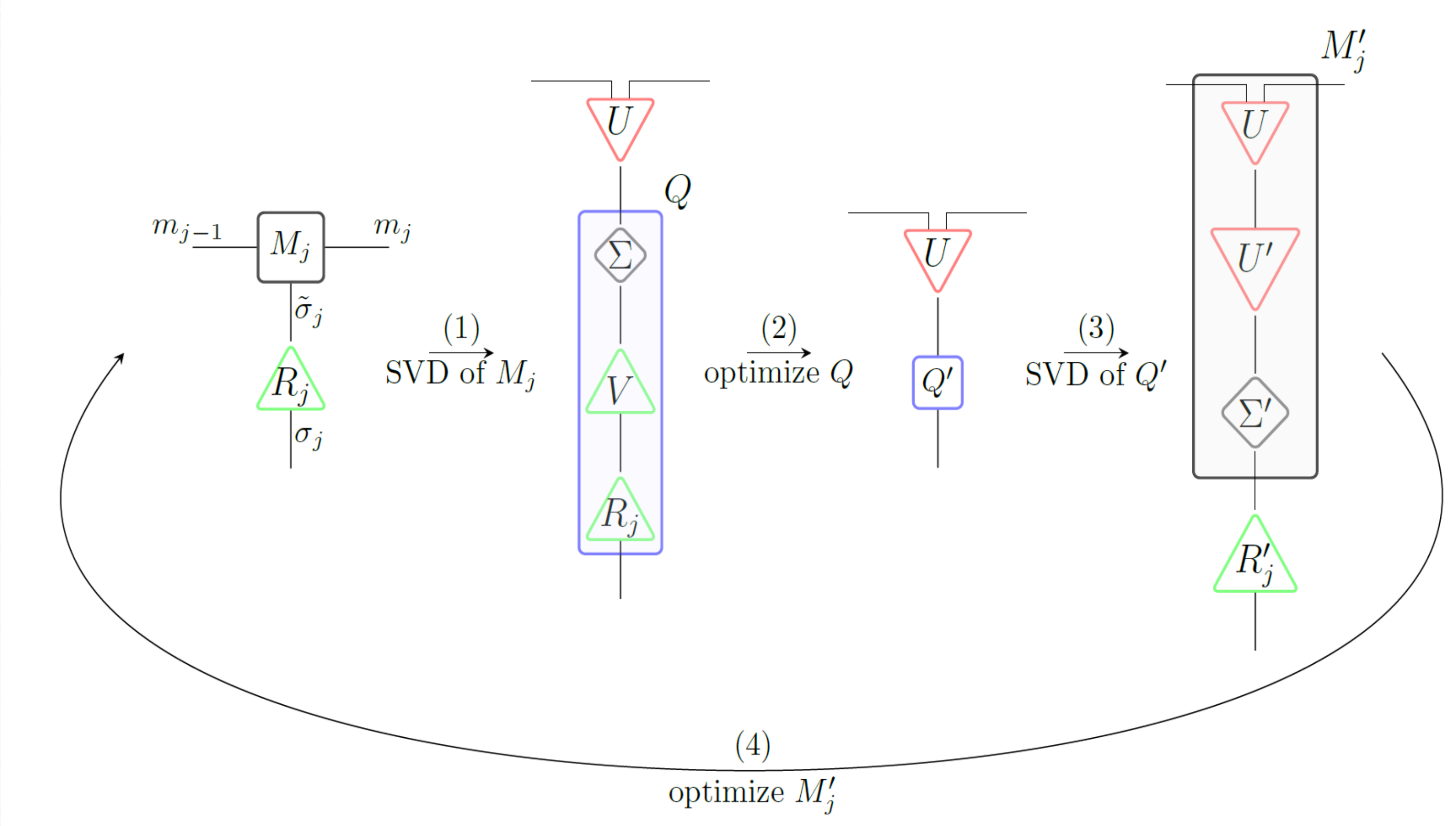
Comparison of these methods: J. Stolpp et al., Comp. Phys. Comm. (2021)

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

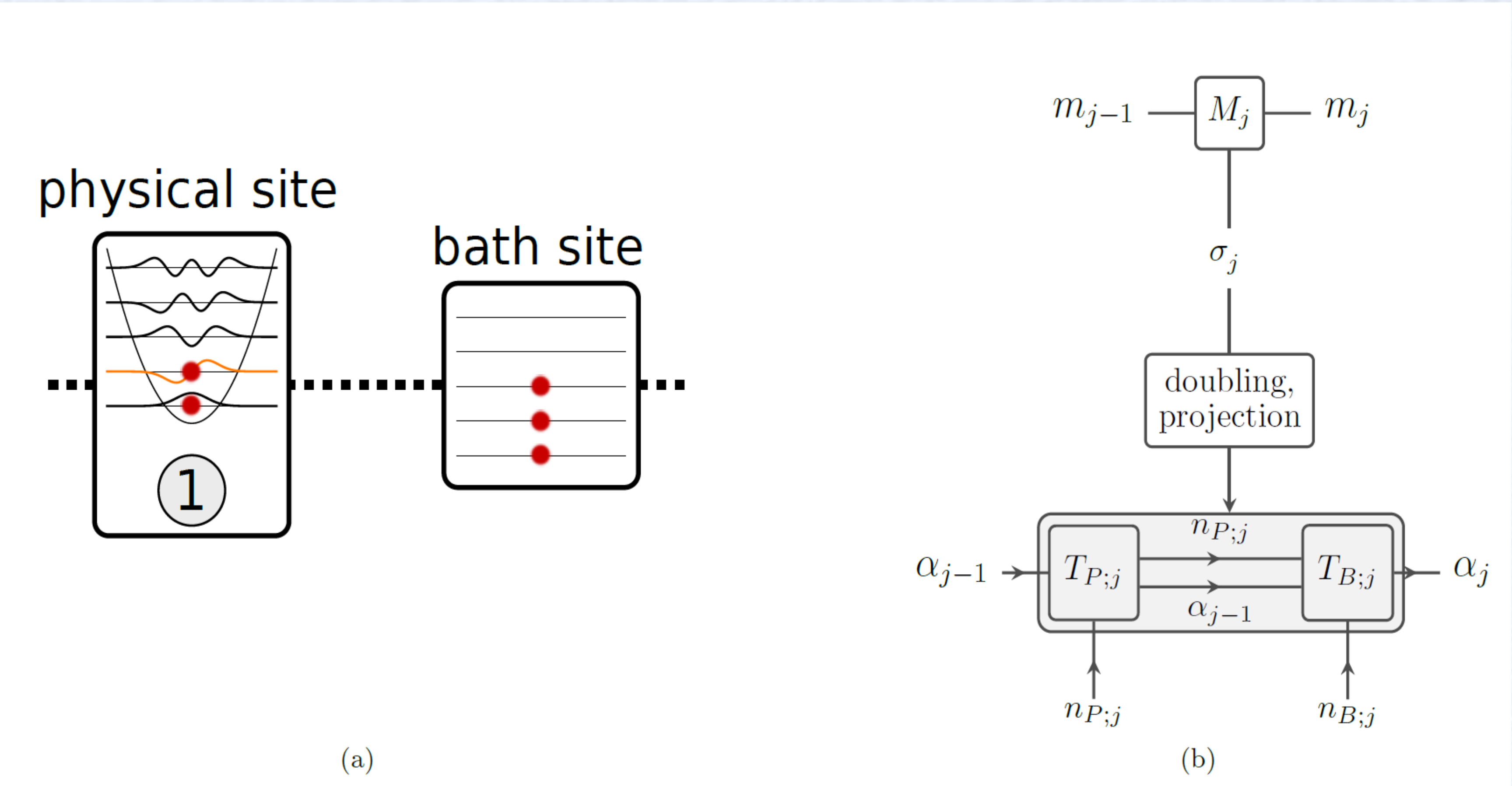


„Pseudo-site approach“ [Jeckelmann & White (1998)]

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



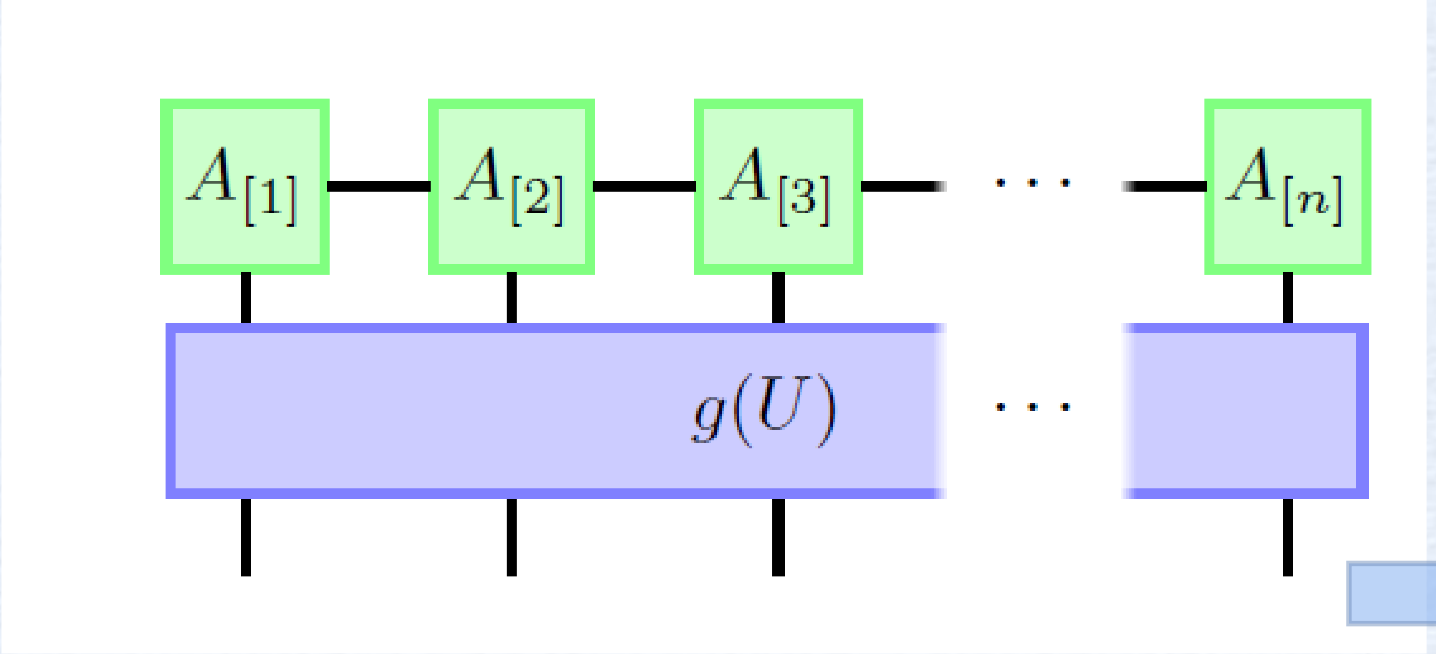
„pp-DMRG“ [T. Köhler, J. Stolpp & S. Paeckel SciPost (2021)]

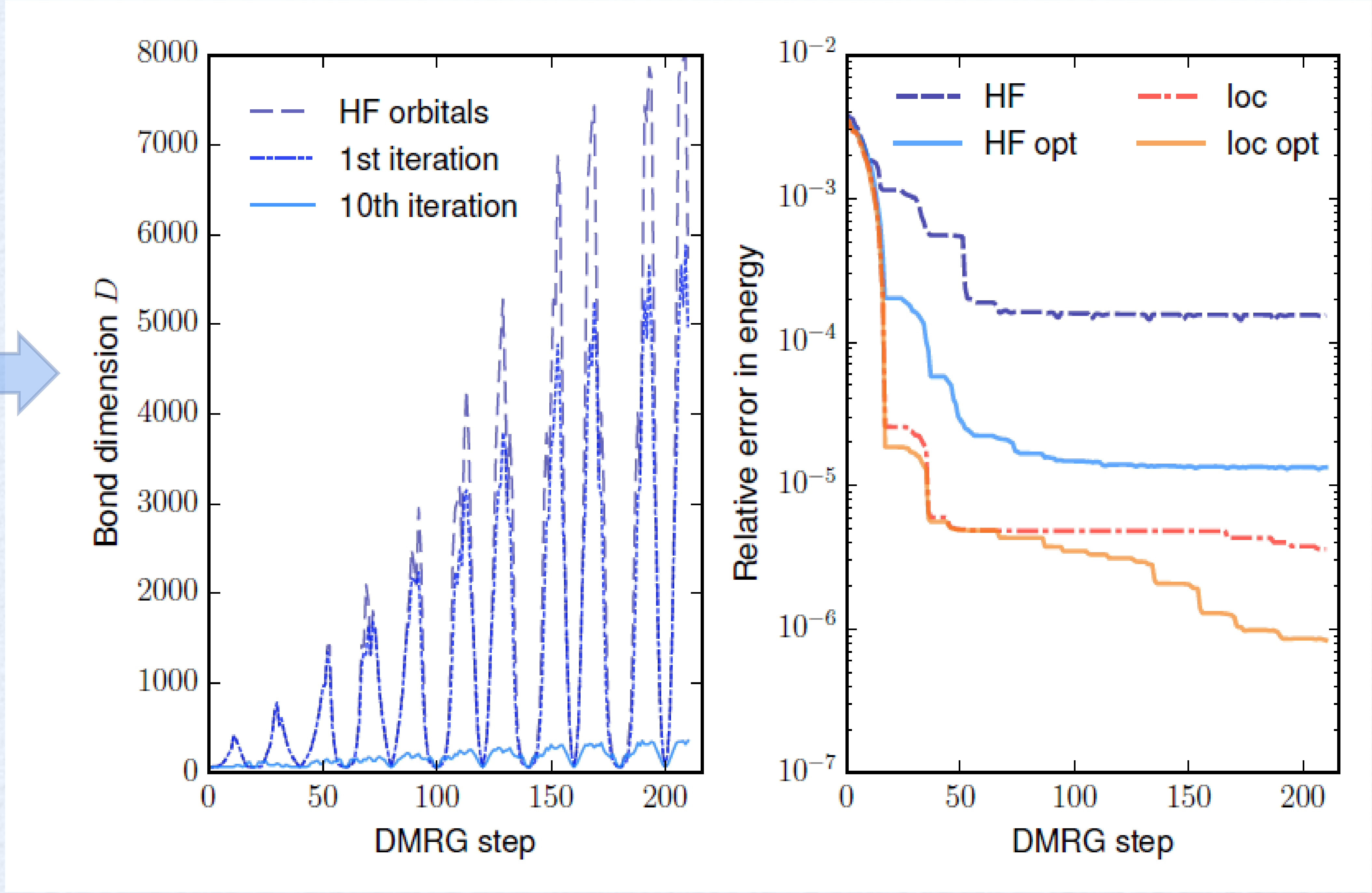


Significantly reduce the entanglement: ‚Mode Optimization‘

[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



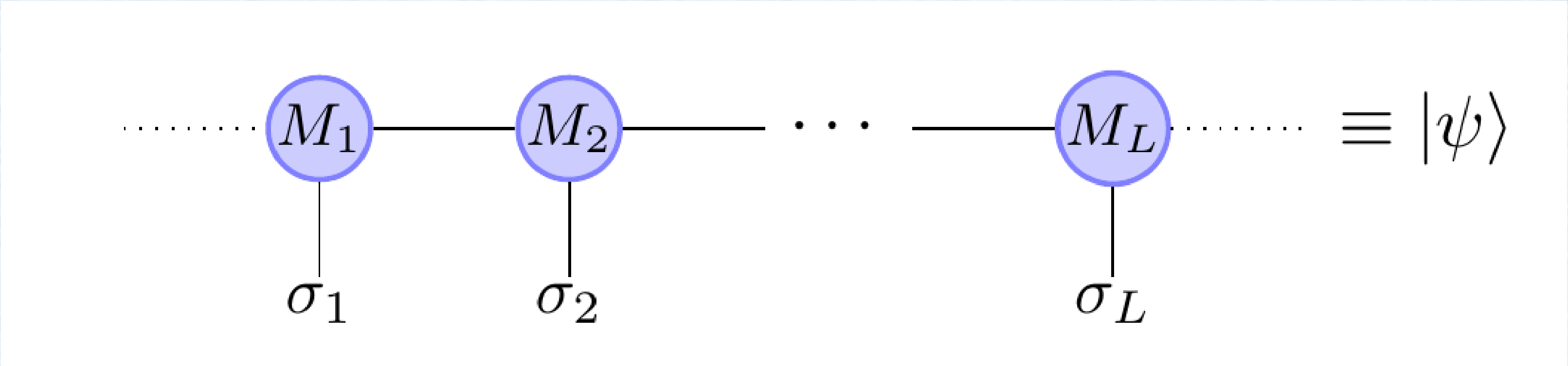


Reduction of the bond dimension from 8000 to ~300 and improvement of the ground state energy!

Conclusions & Outlook

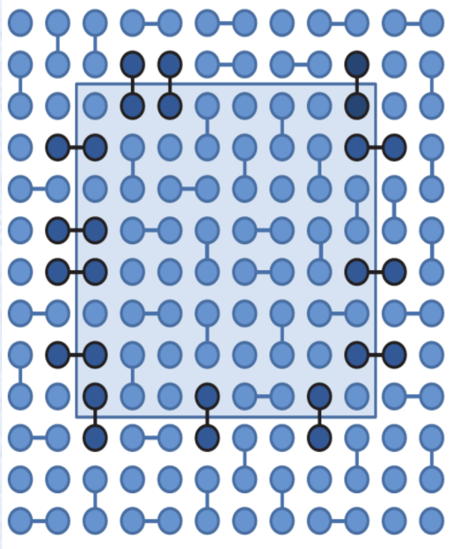
I. Tensor Network methods very flexible and powerful tools:
Basic idea: ‚data compression‘
Ground states, phase diagrams, finite-T, spectral functions, nonequilibrium

II. Specific realization of tensor networks in 1D: MPS/DMRG



III. 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?