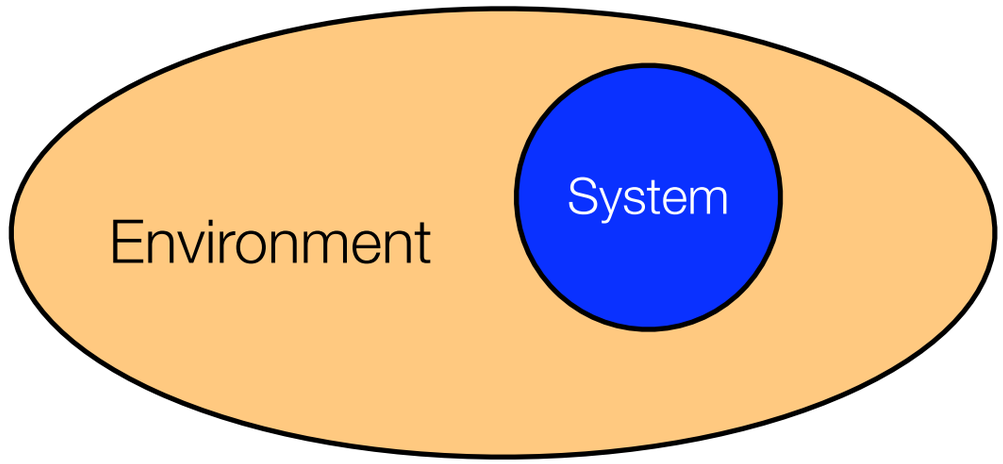


Fourth Lecture:
Density Matrix Renormalization Group et al.

Andreas Läuchli,
“New states of quantum matter”
MPI für Physik komplexer Systeme - Dresden

http://www.pks.mpg.de/~aml
aml@pks.mpg.de

Lecture Notes at http:www.pks.mpg.de/~aml/LesHouches

“Modern theories of correlated electron systems” - Les Houches - 21/5/2009

Outline

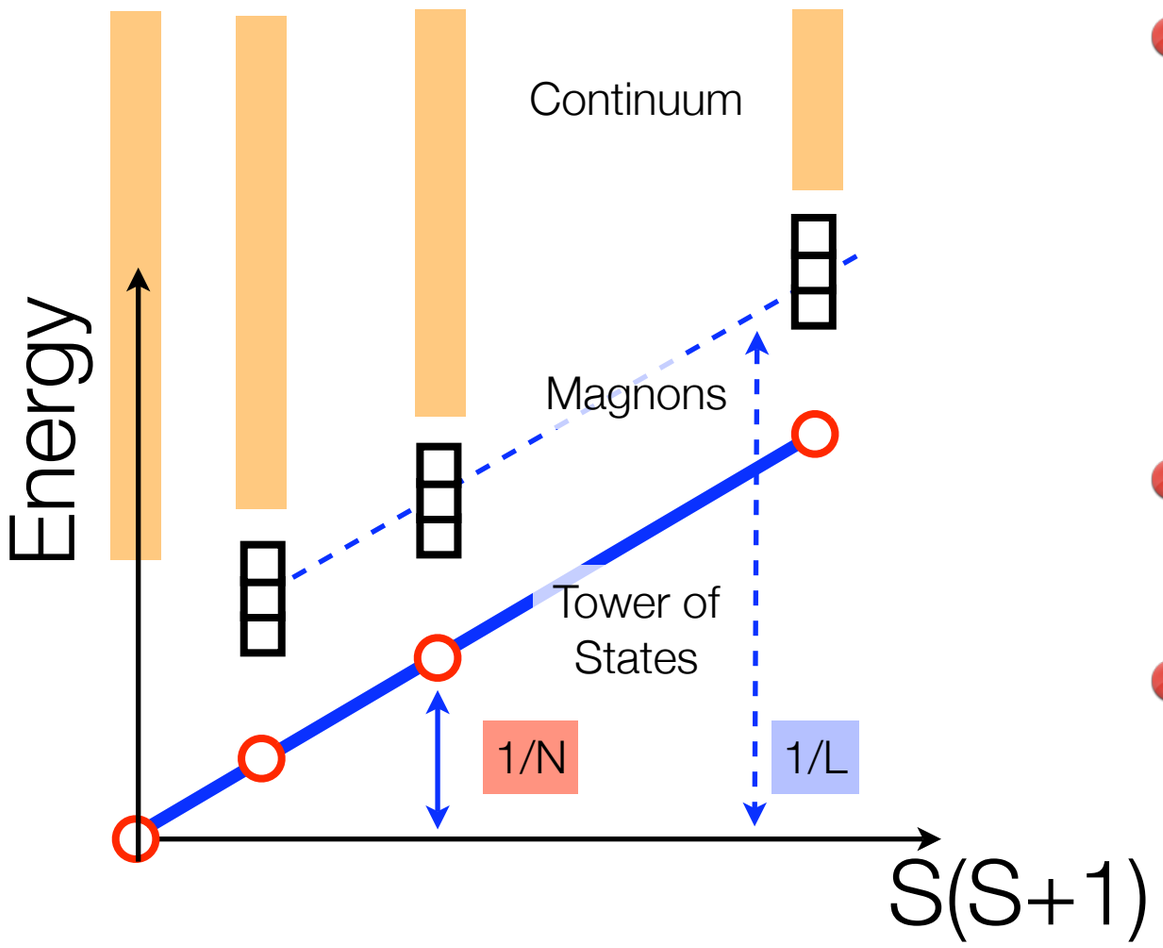
- Tower of States (from yesterday's ED lecture)
- Wilson's RG
- White's DMRG
- What can you do with DMRG ?
  - Ground states, correlation functions
  - Dynamical correlation functions
  - Real-time evolution
  - Classical systems in higher dimension
  - Finite Temperature properties
- DMRG++, MPS, PEPS, MERA, iTEBD, iPEPS

Continuous symmetry breaking and “Tower of States”

“Tower of States” spectroscopy

- What are the finite size manifestations of a continuous symmetry breaking ?

- Low-energy dynamics of the order parameter
  Theory: P.W. Anderson 1952, Numerical tool: Bernu, Lhuillier and others, 1992 -



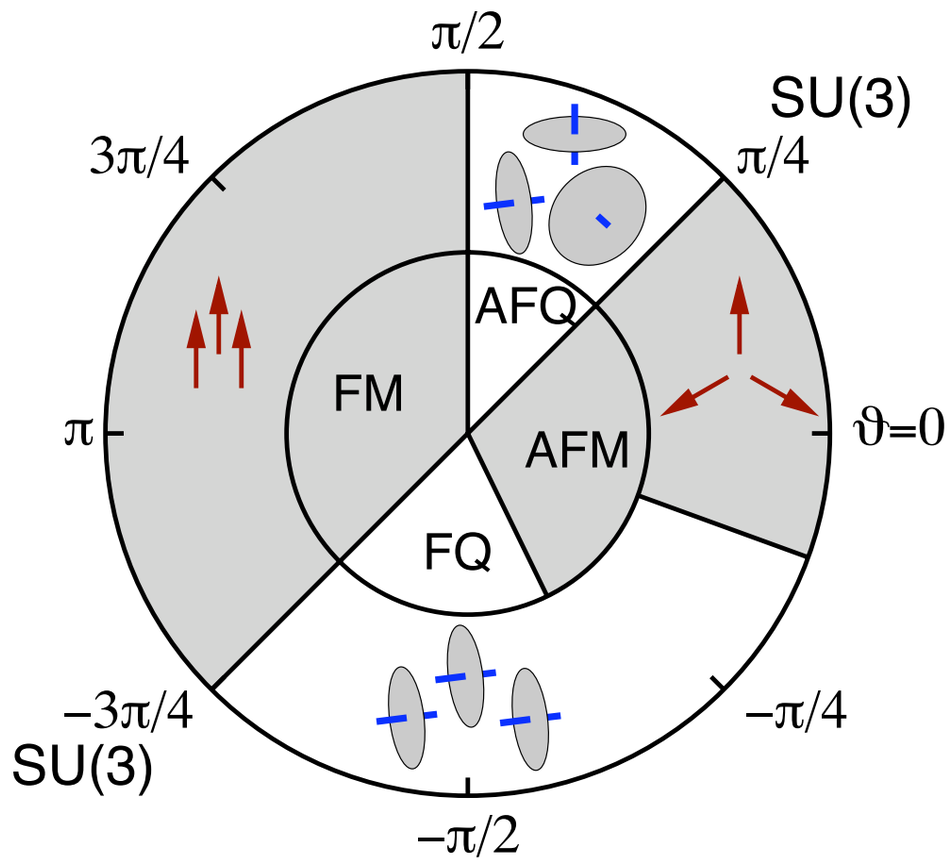
- Dynamics of the free order parameter is visible in the finite size spectrum. Depends on the continuous symmetry group.

- U(1): $(S^z)^2$ SU(2): S(S+1)

- Symmetry properties of levels in the Tower states are crucial and constrain the nature of the broken symmetries.

Tower of States
S=1 on triangular lattice

- Bilinear-biquadratic S=1 model on the triangular lattice (model for $NiGaS_4$).

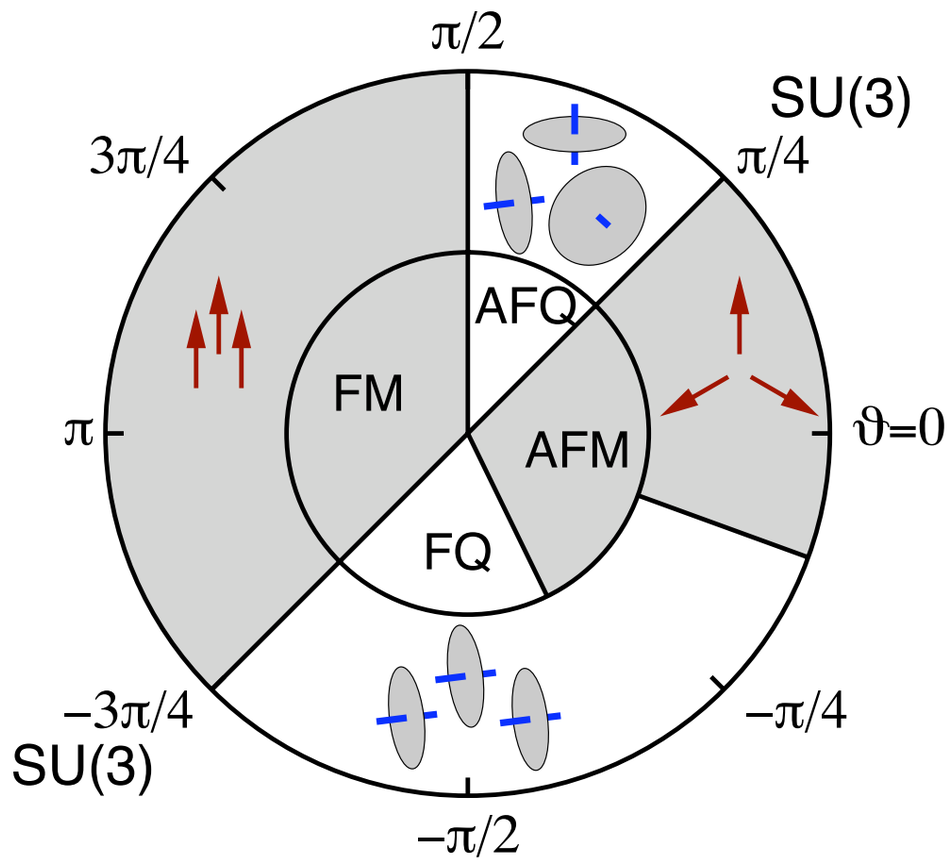


AML, F. Mila, K. Penc, PRL ‘06

Tower of States
S=1 on triangular lattice

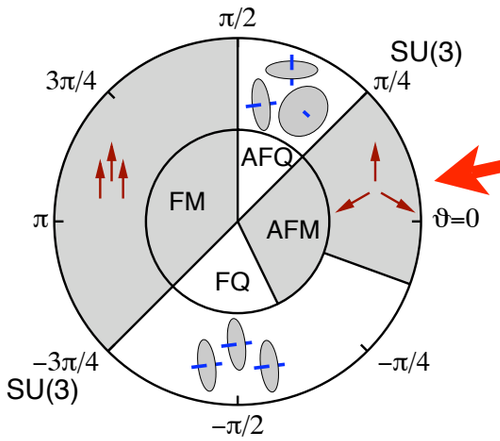
- Bilinear-biquadratic S=1 model on the triangular lattice (model for $NiGaS_4$).

$$H = \sum_{\langle i,j \rangle} \cos(\theta)\ \mathbf{S}_i \cdot \mathbf{S}_j + \sin(\theta)\ \ (\mathbf{S}_i \cdot \mathbf{S}_j)^2$$

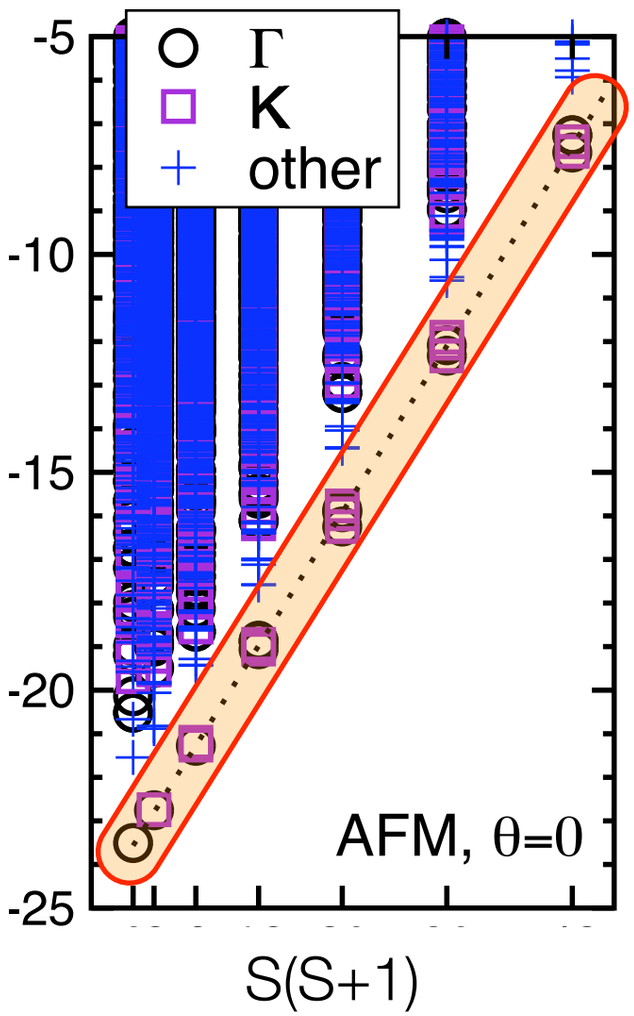


AML, F. Mila, K. Penc, PRL '06

Tower of States
S=1 on triangular lattice: Antiferromagnetic phase

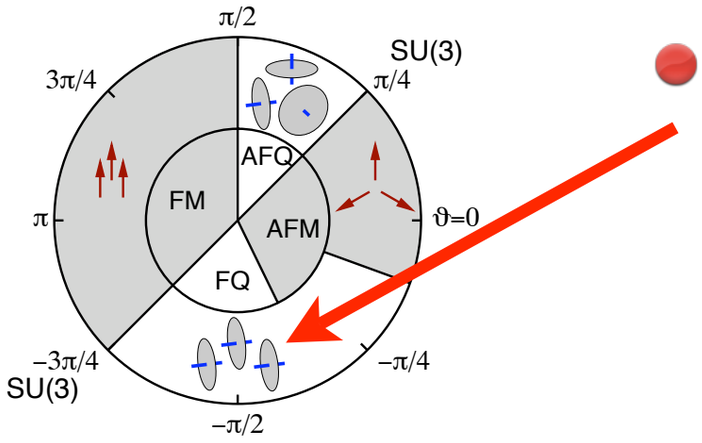


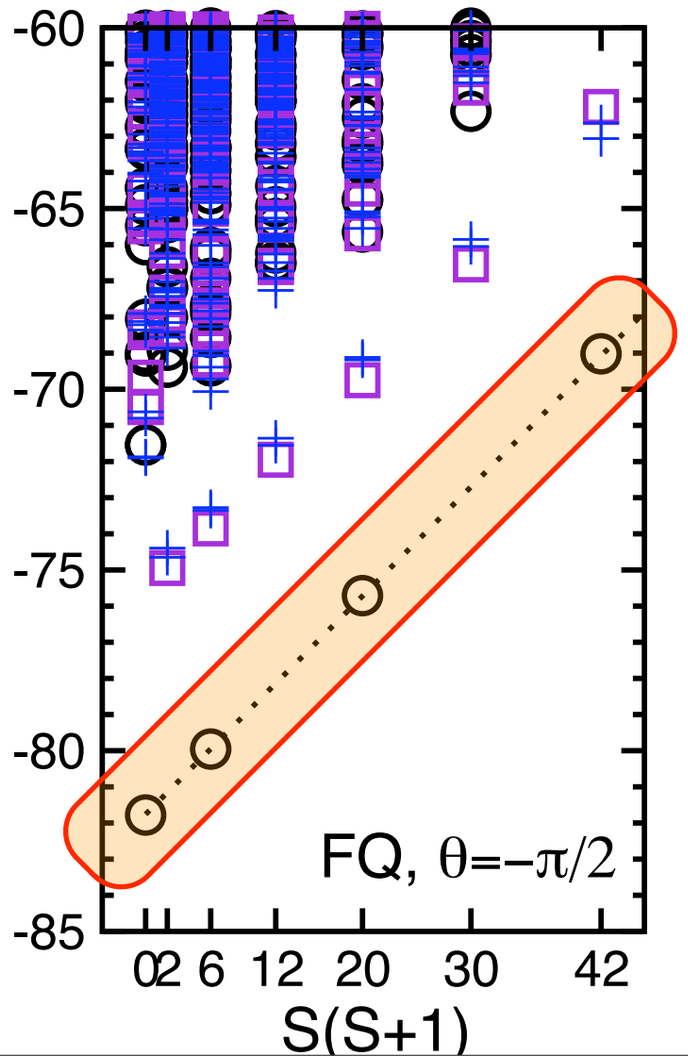
- ϑ=0 : coplanar magnetic order,
  120 degree structure



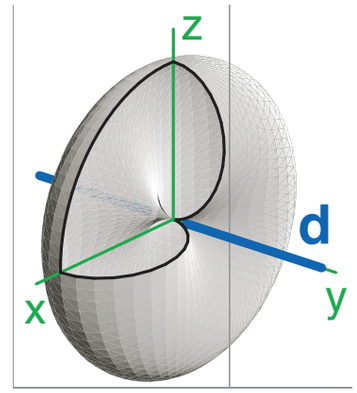
- Breaks translation symmetry. Tree site unit cell
  ⇒ nontrivial momenta must appear in TOS
- non-collinear magnetic structure
  ⇒ SU(2) is completely broken,
  number of levels in TOS increases with S
- Quantum number are identical to the S=1/2 case

Tower of States
S=1 on triangular lattice: Ferroquadrupolar phase





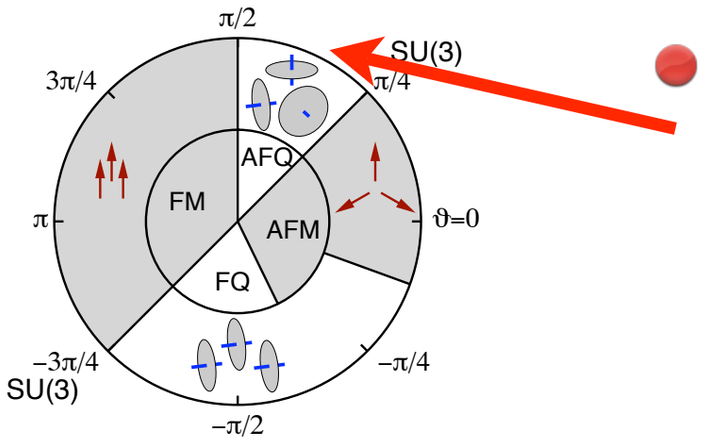
- ϑ=-π/2 : ferroquadrupolar phase, finite quadrupolar moment, no spin order



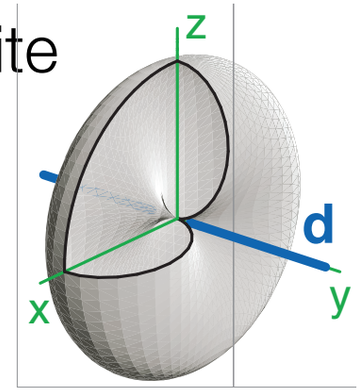
- No translation symmetry breaking.
  ⇒ only trivial momentum appears in TOS
- Ferroquadrupolar order parameter, only even S
- all directors are collinear
  ⇒ SU(2) is broken down to U(1),

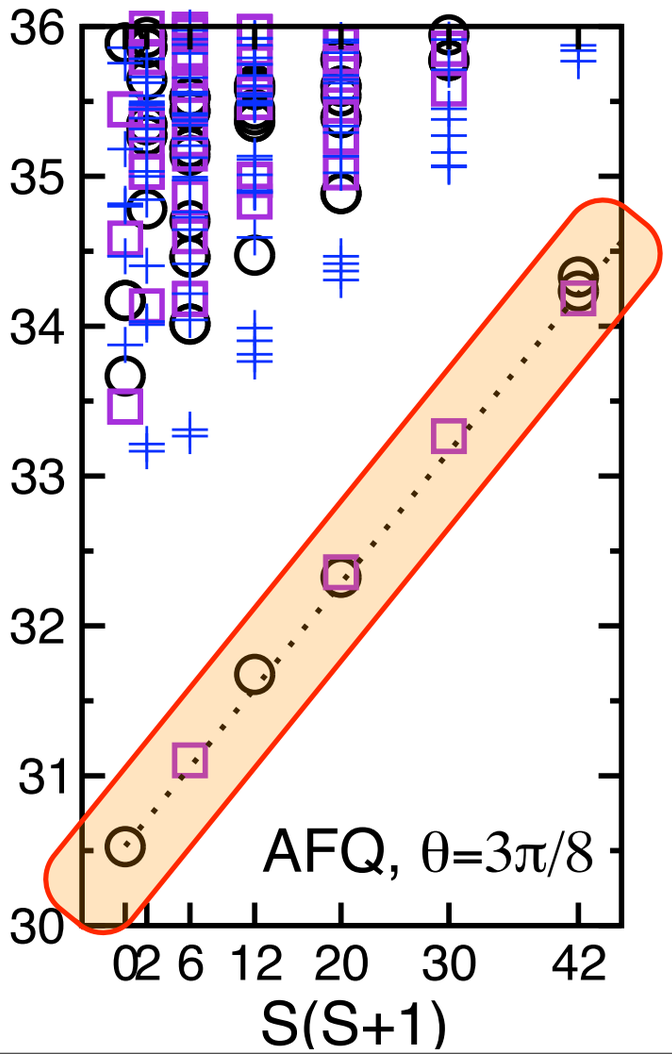
  number of states in TOS is independent of S.

Tower of States
S=1 on triangular lattice: Antiferroquadrupolar phase



- ϑ=3π/8 : antiferroquadrupolar phase, finite quadrupolar moment, no spin order, three sublattice structure.





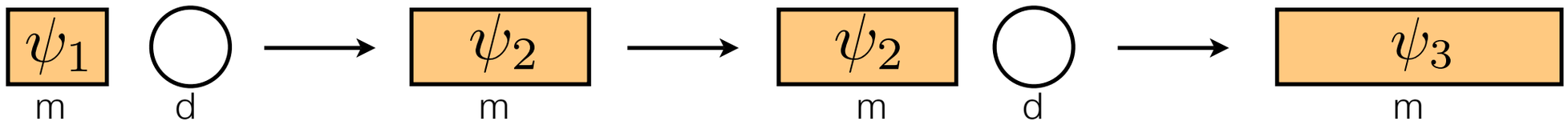
- Breaks translation symmetry. Tree site unit cell ⇒ nontrivial momenta must appear in TOS

- Antiferroquadrupolar order parameter, complicated S dependence. Can be calculated using group theoretical methods.

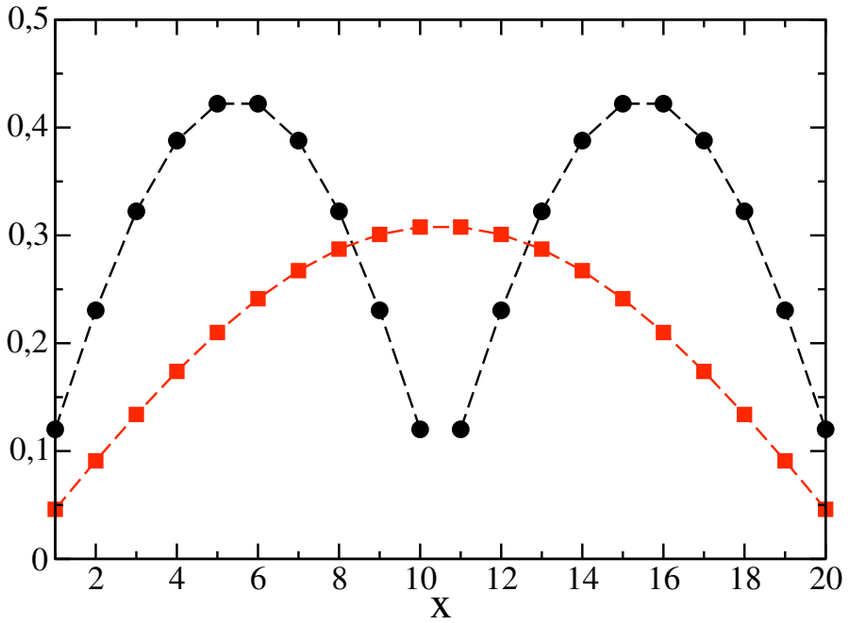
Density Matrix Renomalization Group et al.

Density Matrix Renormalization Group

- K. Wilson introduced the numerical renormalization group as a powerful numerical tool to solve the Kondo problem (Wilson RMP 75).



- Many people tried to apply this idea in a straightforward way to quantum many body problems and failed. The reason for this failure was understood in a study of the tight-binding problem on a chain (White & Noack PRL 92):



$$\psi[2L] \neq \psi[L] \otimes \psi[L]$$

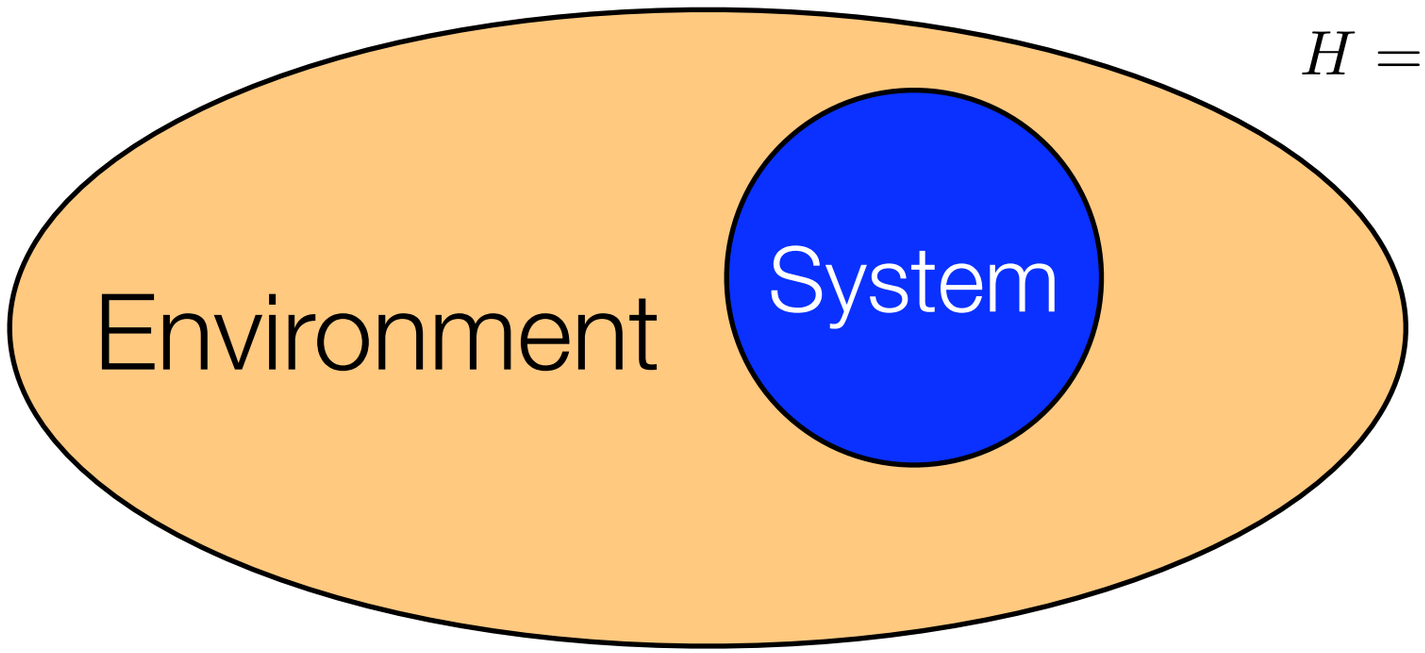
The groundstate of the large system is not at all well approximated by the tensor product of the groundstates of the smaller systems

Density Matrix Renormalization Group

- The next crucial step was to realize how one has to choose the states to be kept in a partition of the universe:

$$H = H_S + H_E + H_{SE}$$

groundstate $|\psi\rangle$



- System description with *m* states:

$$|\tilde{\psi}\rangle = \sum_{n}^{m} \sum_{\alpha} \tilde{\psi}_{n,\alpha} |\phi_n\rangle_S \otimes |\alpha\rangle_E$$

- How to choose the *m* states in order to approximate $|\psi\rangle$ best ?

Density Matrix Renormalization Group

- The answer is given by the subsystem density matrix

$$\rho_{i,j} = \mathrm{Tr}_E |\psi\rangle\langle\psi|$$

- With the help of the Schmidt decomposition one can show that the *m* eigenfunctions of ρ associated with the largest eigenvalues w_n give the best approximation of $|\psi\rangle$. (and not the lowest eigenstates of H_S)

- The error can be estimated to be

$$\left| |\tilde{\psi}\rangle - |\psi\rangle \right|^2 \approx 1 - \sum_n^m w_n = P_m$$

Density Matrix Renormalization Group

Density Matrix Renormalization Group

- Based on these condsiderations, S.R. White came up with the DMRG
  S.R. White, PRL **69**, 2863 (1992); PRB **48**,10345 (1993).

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- Infinite System Algorithm

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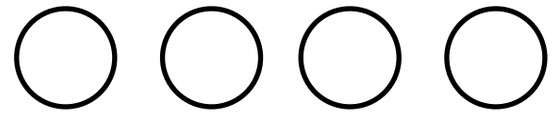

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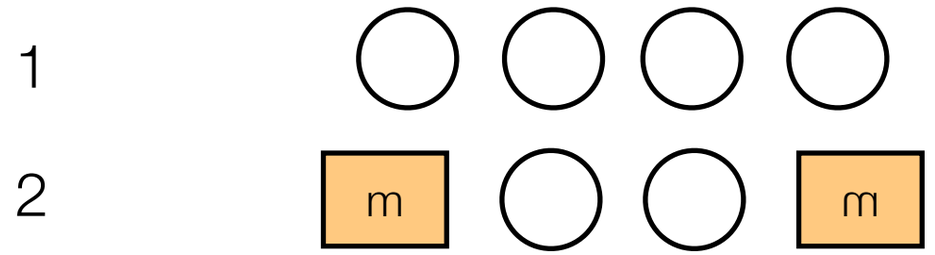

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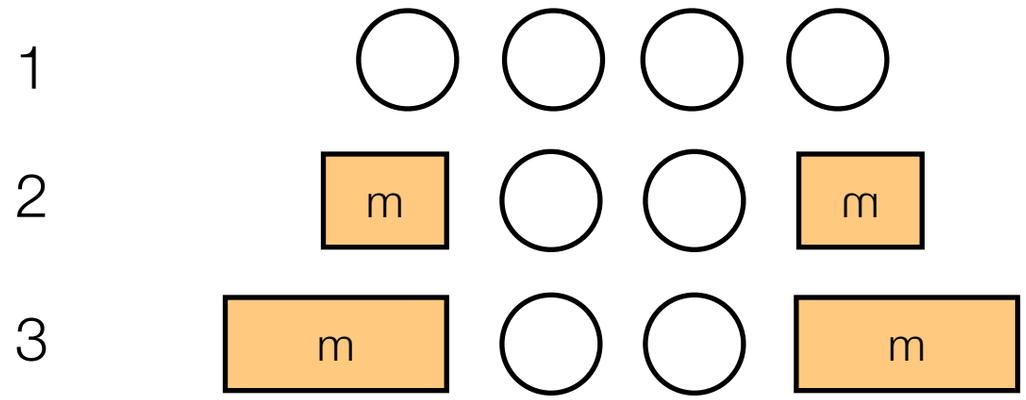

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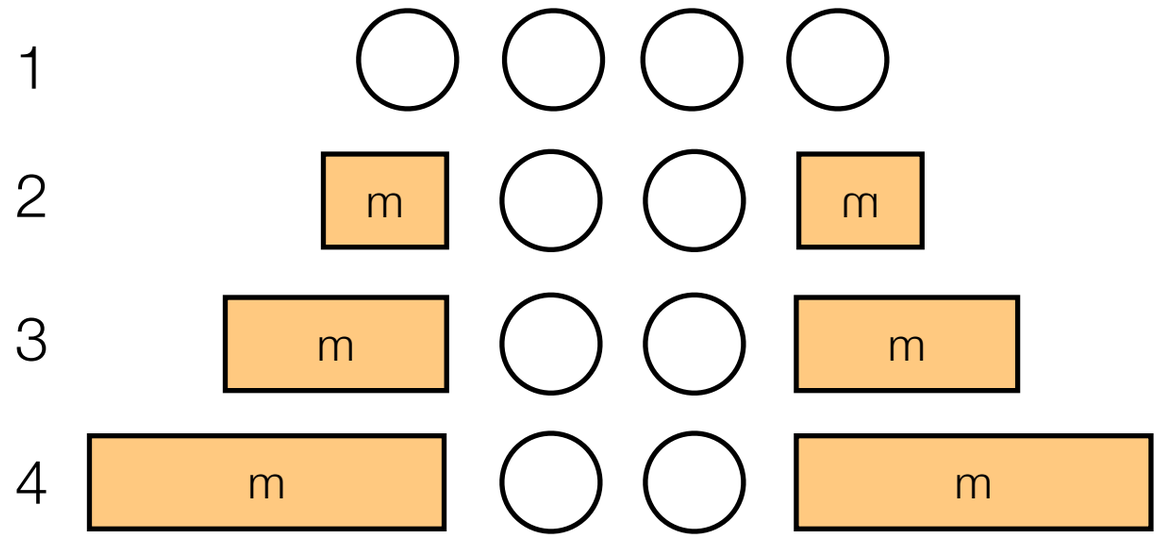

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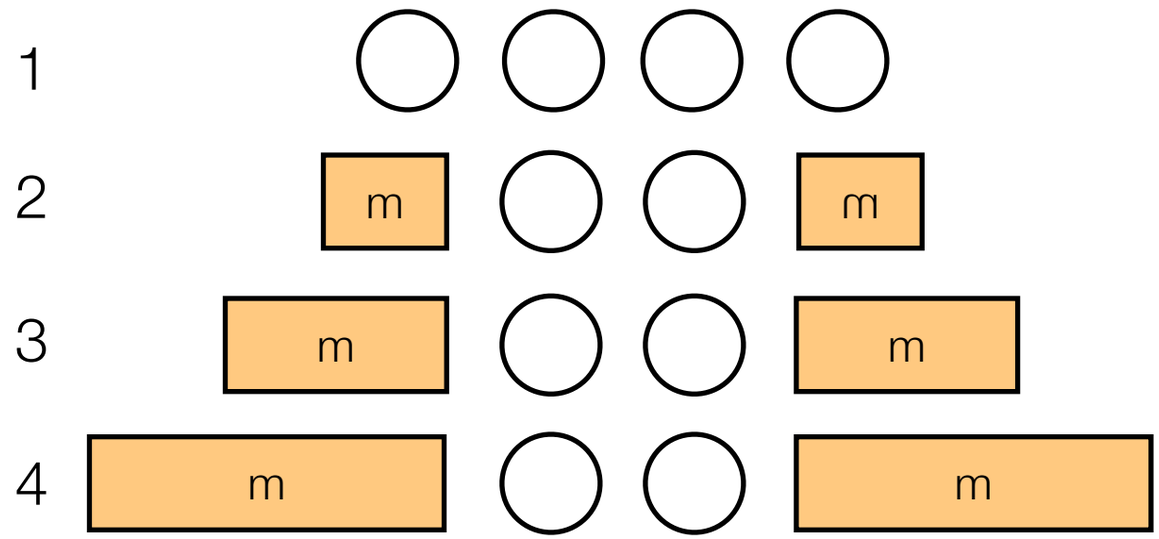

- Finite System Algorithm

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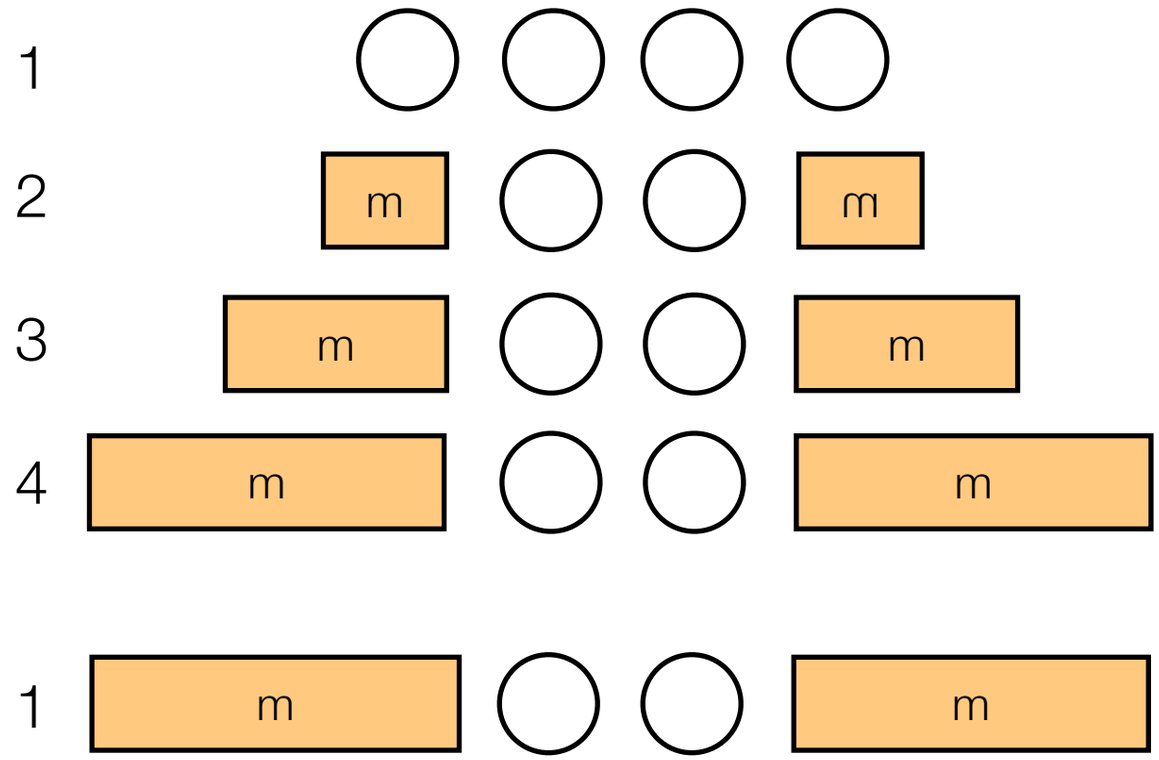

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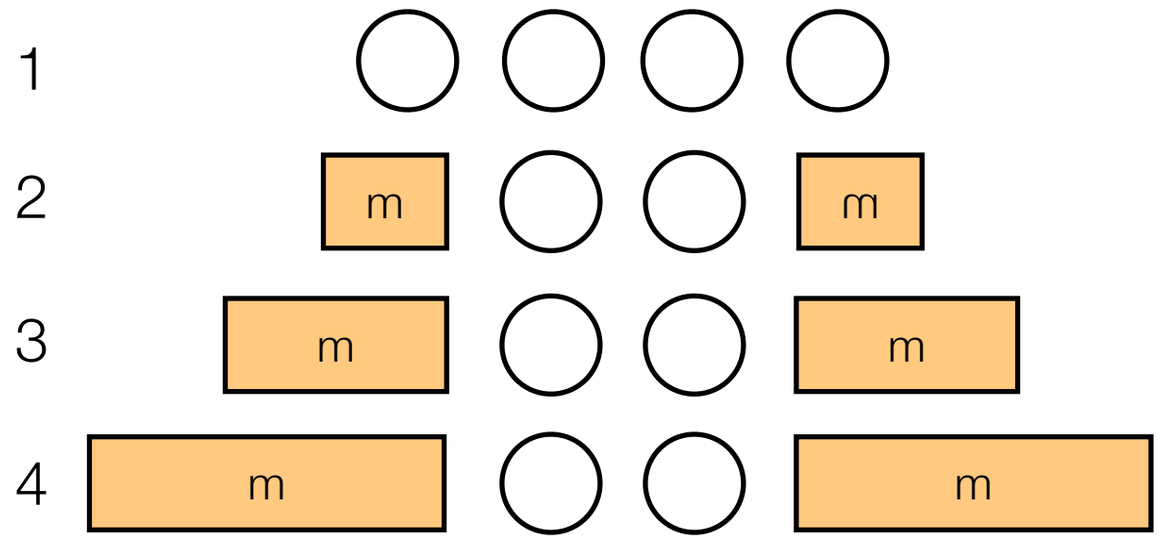

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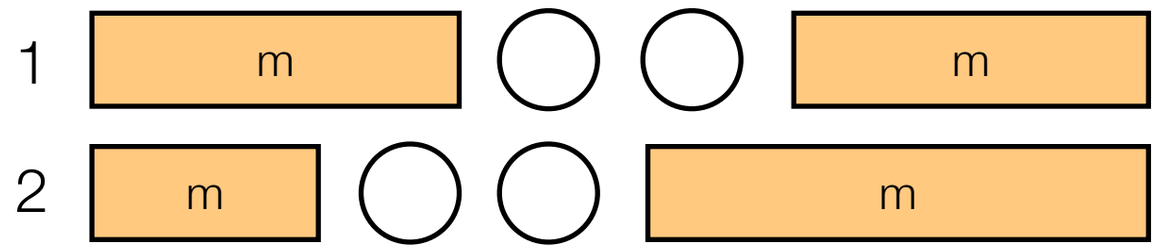

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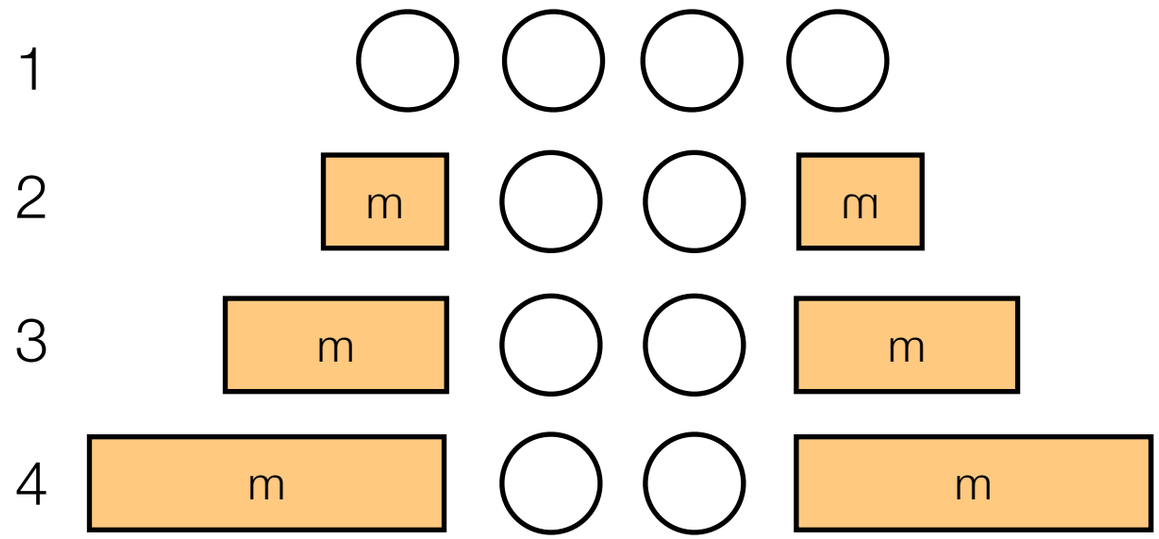

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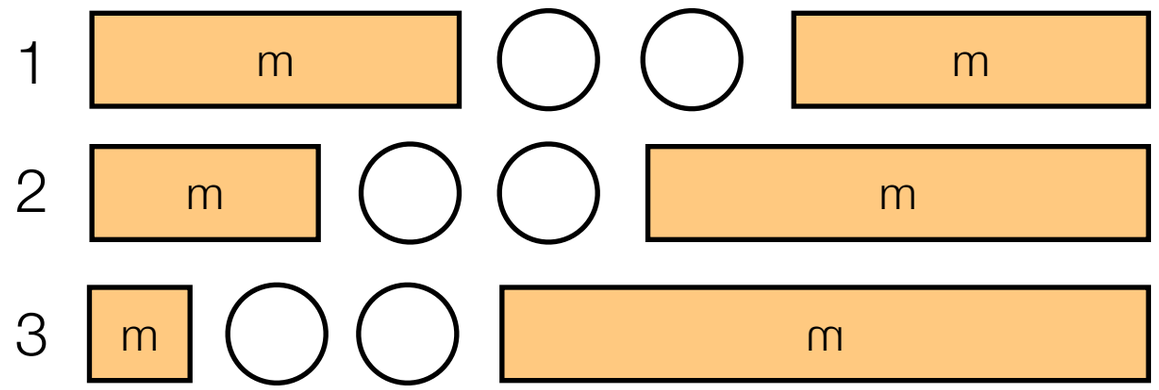

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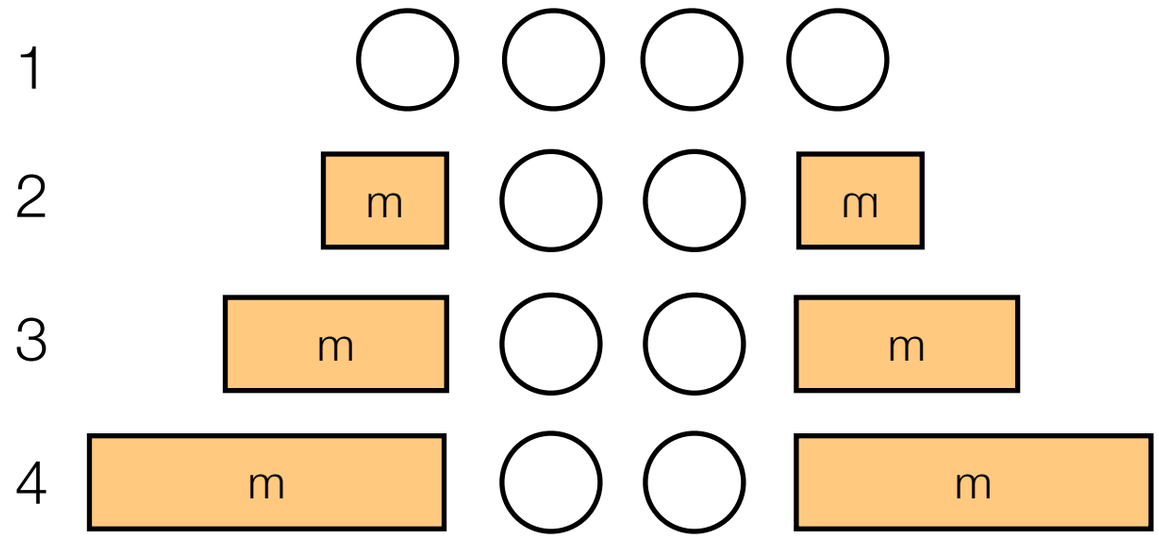

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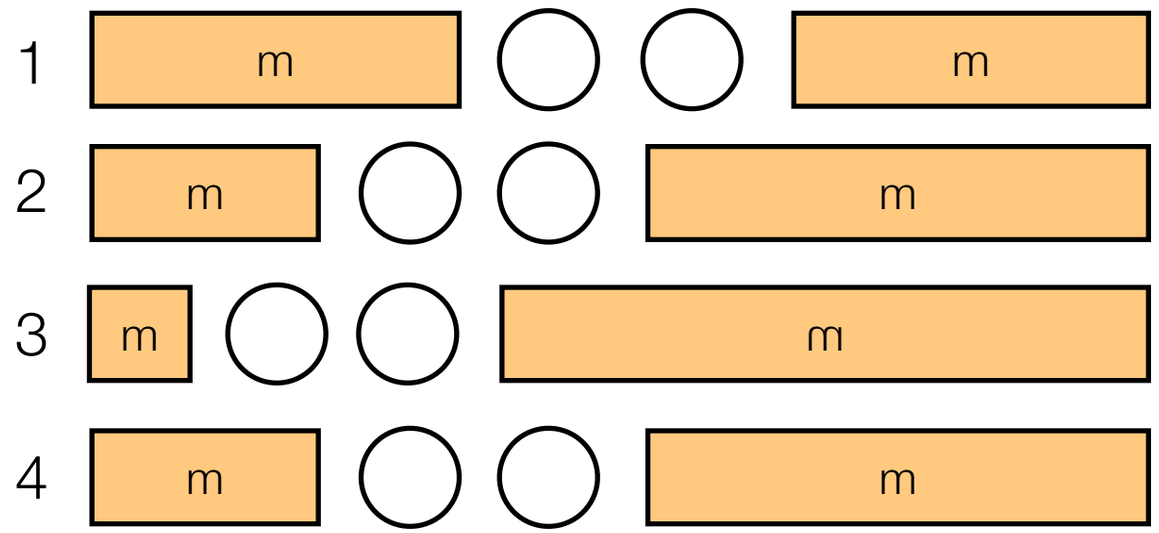


Applicability of ground state DMRG

- Very efficient groundstate simulations for many 1D systems.
  Frustration or fermions pose no particular problem.

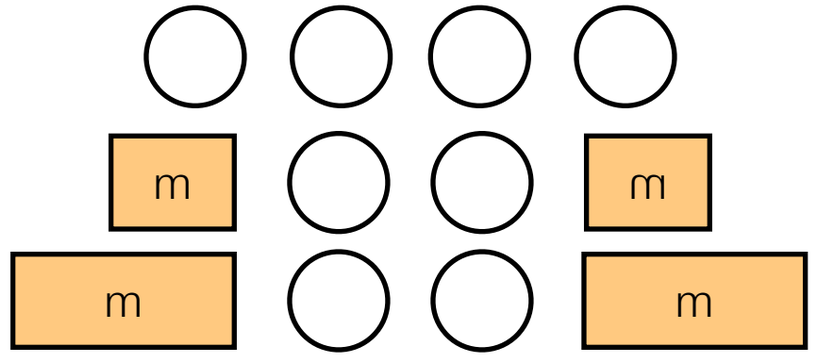
- Typical system sizes and number of states:
  simple spin systems: 100-1000 sites, lower hundred states
  complicated spin systems: hundred sites, larger hundred to thousand states
  fermionic systems, wide systems, many low energy states, they all increase *m*

- Variational, quasi-exact method.

- Wavefunction method, therefore many observables are easily available.

- Drawbacks: it is not yet possible to simulate very large 2D systems,
  open boundaries might not always be what we desire, especially
  because of the lack of spatial quantum numbers.

Infinite System Algorithm in Detail



1. Form a superblock containing L sites which is small enough to be exactly diagonalized

2. Diagonalize the superblock Hamiltonian H_L^{super} numerically, obtaining only the ground state eigenvalue and eigenvector $|\psi\rangle$ using Lanczos or Davidson.

3. Form the reduced density matrix $\rho_{ii'}$ for the new system block from $|\psi\rangle$ using $\rho_{ii'} = \sum_j \psi^*_{ij}\psi_{i'j}$.

4. Diagonalize $\rho_{ii'}$ with a dense matrix diagonalization routine to obtain the m eigenvectors with the largest eigenvalues

5. Construct H_{l+1} and other operators in the new system block and transform them to the reduced density matrix eigenbasis using $\bar{H}_{l+1} = O_L^\dagger H_{l+1} O_L$ where the columns of O_L contain the the m highest eigenvectors of $\rho_{ii'}$.

6. Form a superblock of size L+2 using $\bar{H}_{l+1}$, two single sites and $\bar{H}^R_{l+1}$.

7. Repeat starting with step 2, substituting H^{super}_{L+2} for H^{super}_L.

Efficiency

- Efficient multiplication of H_L^{super} with a vector is important. Wave function transformation yields significant speedup.

- Computational cost: L m^3
  Memory cost: (L) m^2

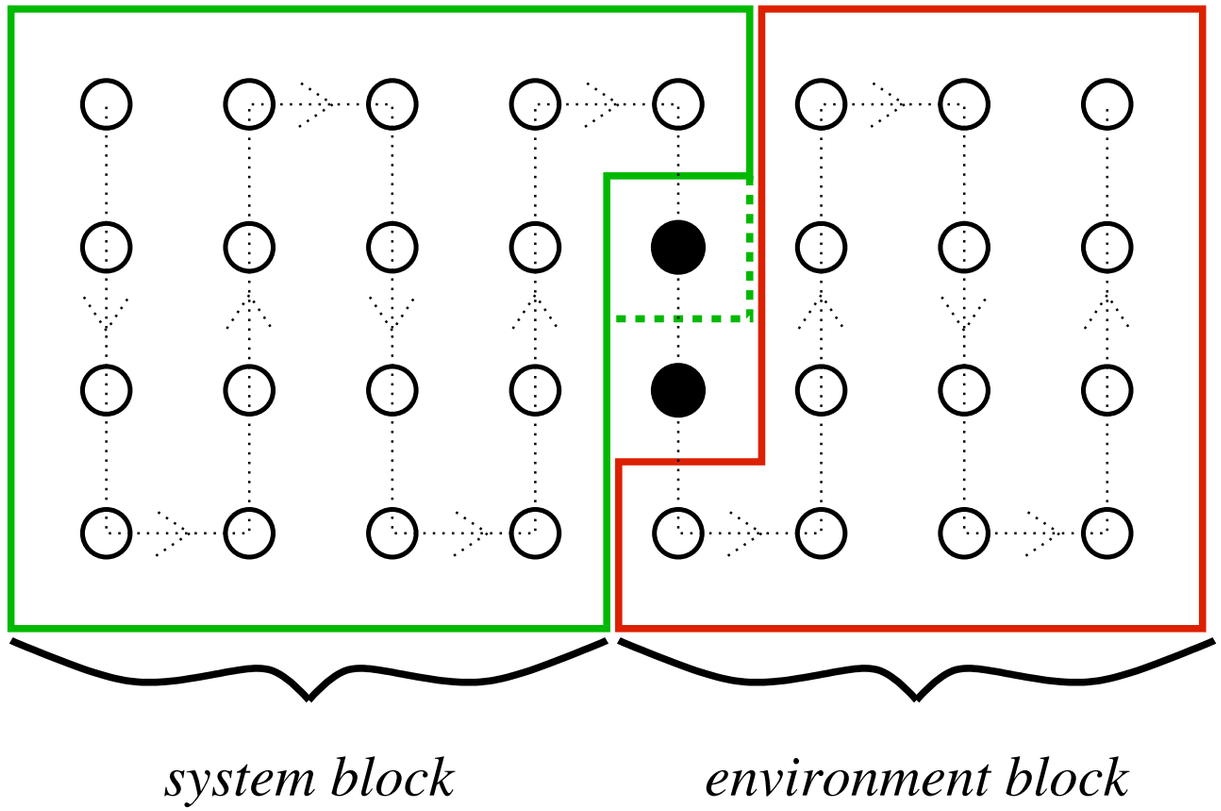
- Abelian quantum numbers Np and Sz can be implemented. They render the matrices block sparse, but require book keeping effort.

- Nonabelian quantum numbers [e.g. S(S+1)] can be implemented, but gives more complex code.

- Writing to disk. Information not needed at the current step can be stored on disk.

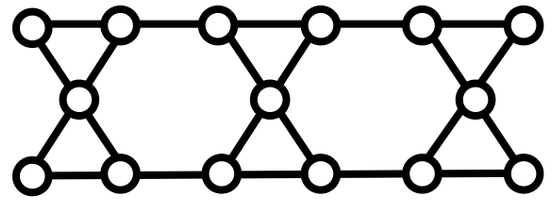
Extension to ladder systems

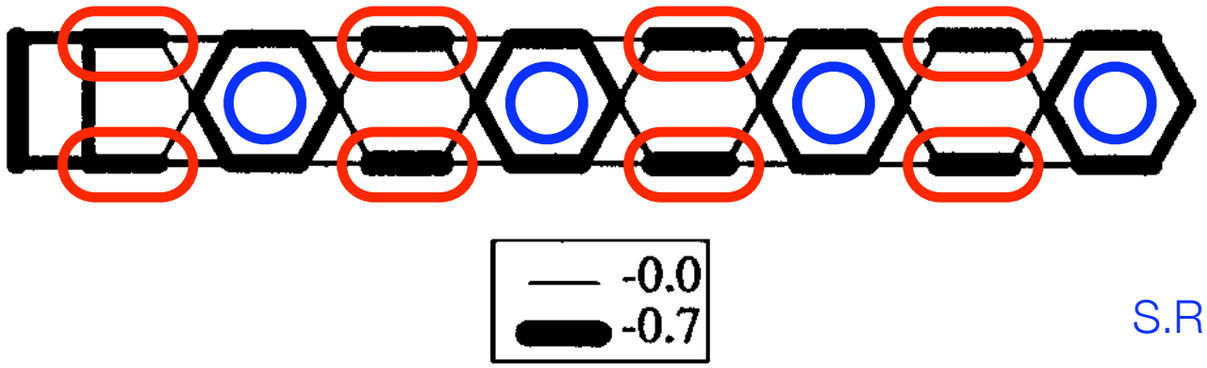
- 1D algorithm folded into 2D
- finite size algorithm needed
- Convergence depends strongly on width of system
- Exponential effort in width for spinless fermions



DMRG Applications
The S=1/2 Kagome Strips

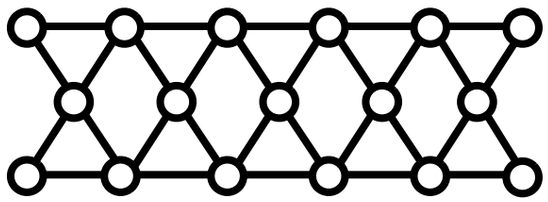
1st Kagome Strip (Azaria et al, 1998)



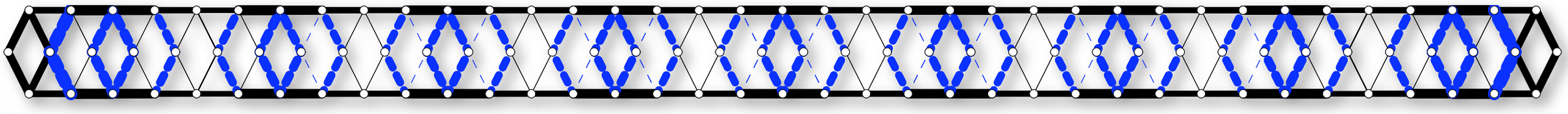


S.R. White & R.R.P. Singh PRL (2000)

2nd Kagome Strip (Waldtmann, Everts et al, 2000)

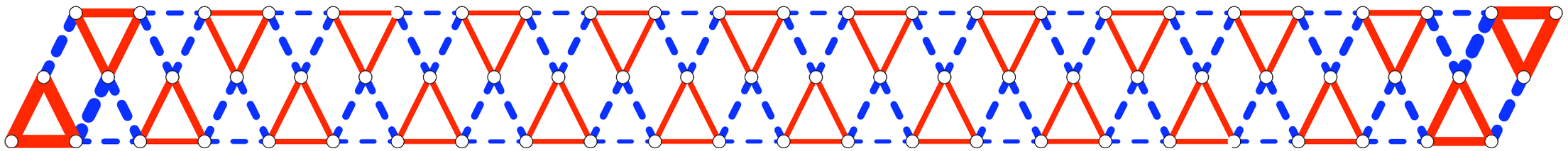


undoped, Heisenberg model



AML, unpublished

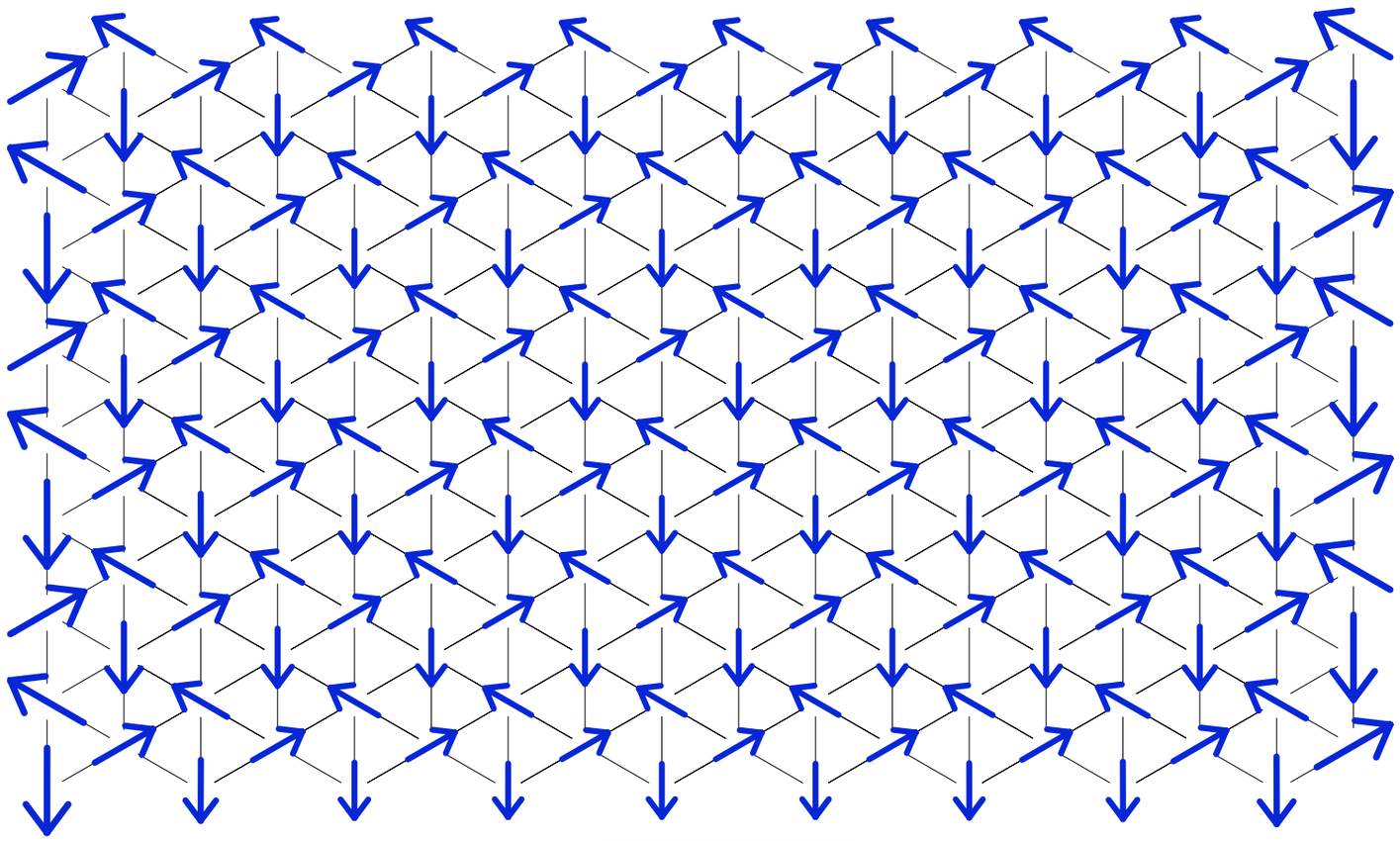
doped <n>=2/3 → 3 site singlets

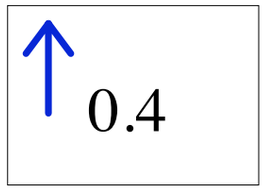


M. Indergand, AML, S. Capponi, M.Sigrist, PRB (2006)

DMRG Applications
Triangular lattice Heisenberg model

- Very accurate determination of order parameter using special aspect ratio to suppress leading finite size corrections.





$\Delta E \sim 0.3\%, \quad \Delta \langle S_z \rangle \sim 0.01$

See White & Chernyshev, PRL 99, 127004 (2007)

Extensions:
Dynamical DMRG (D-DMRG)

- Dynamical correlation function

$$G(\mathbf{k}, \omega = \langle \psi_0 | A_{\mathbf{k}}^\dagger (\omega + i\eta - H)^{-1} A_{\mathbf{k}} | \psi_0 \rangle$$

  additional density matrix eigenstates must be “targeted”

- Lanczos vector method: target Krylov vectors (Hallberg 1995)

$$|\psi_0\rangle,\ A_{\mathbf{k}}^\dagger|\psi_0\rangle,\ H A_{\mathbf{k}}^\dagger|\psi_0\rangle,\ H^2 A_{\mathbf{k}}^\dagger|\psi_0\rangle,\ \ldots$$

- Correction vector method: target vectors: (White & Kuehner 1999)

$$|\psi_0\rangle,\ A_{\mathbf{k}}^\dagger|\psi_0\rangle,\ (\omega + i\eta - H)^{-1} A_{\mathbf{k}}^\dagger|\psi_0\rangle$$

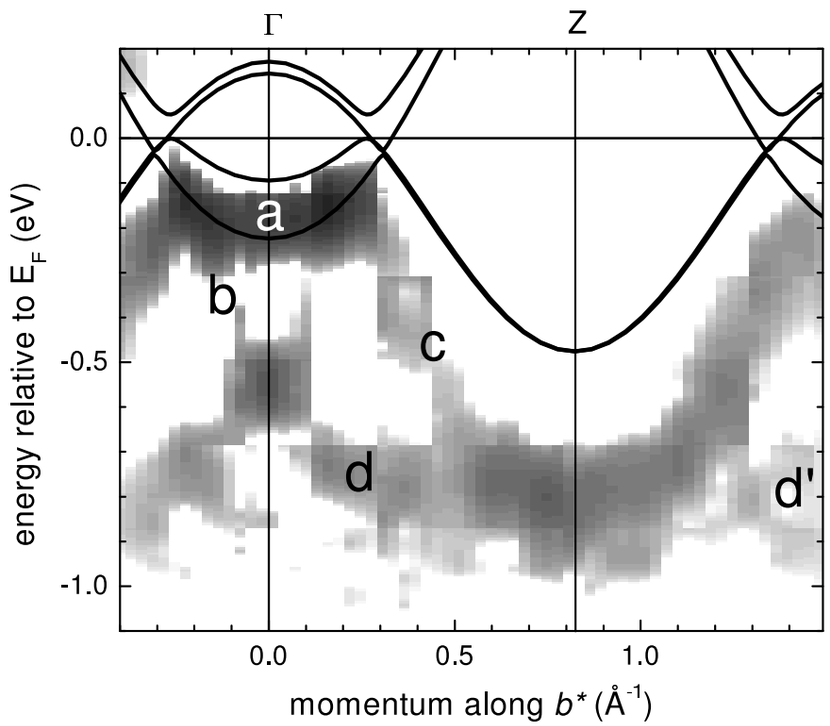
  more accurate than Lanczos vector method, but requires new run for each ω

- Minimization method (DDMRG) (Jeckelmann 2002)
  correction vector minimizes certain functional and value of functional at minimum is the requested spectral weight. more accurate than correction vector

D-DMRG:
Example for photoemission spectrum

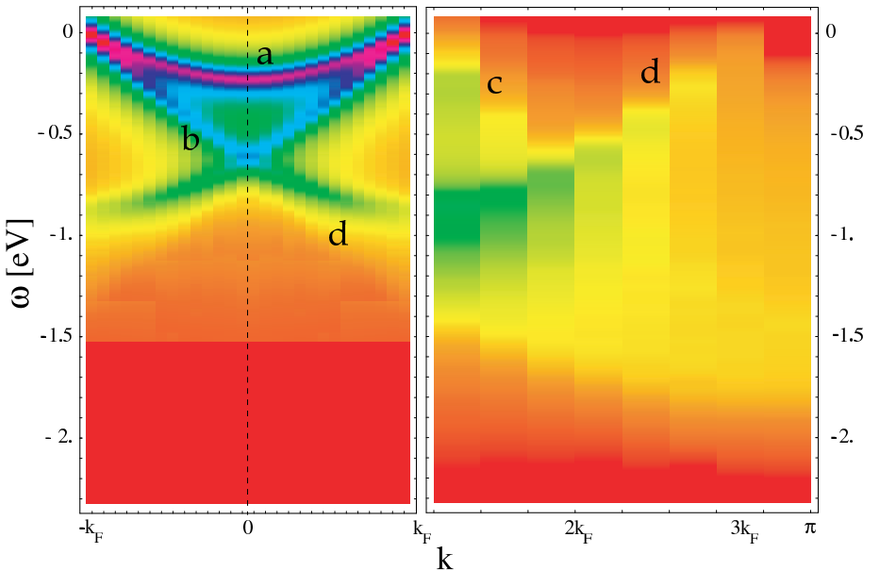
Comparison with ARPES on TTF-TCNQ

ARPES



(Sing *et al., 2003*)

DDMRG



(Benthien et al 2004)

Time dependent DMRG (t-DMRG)

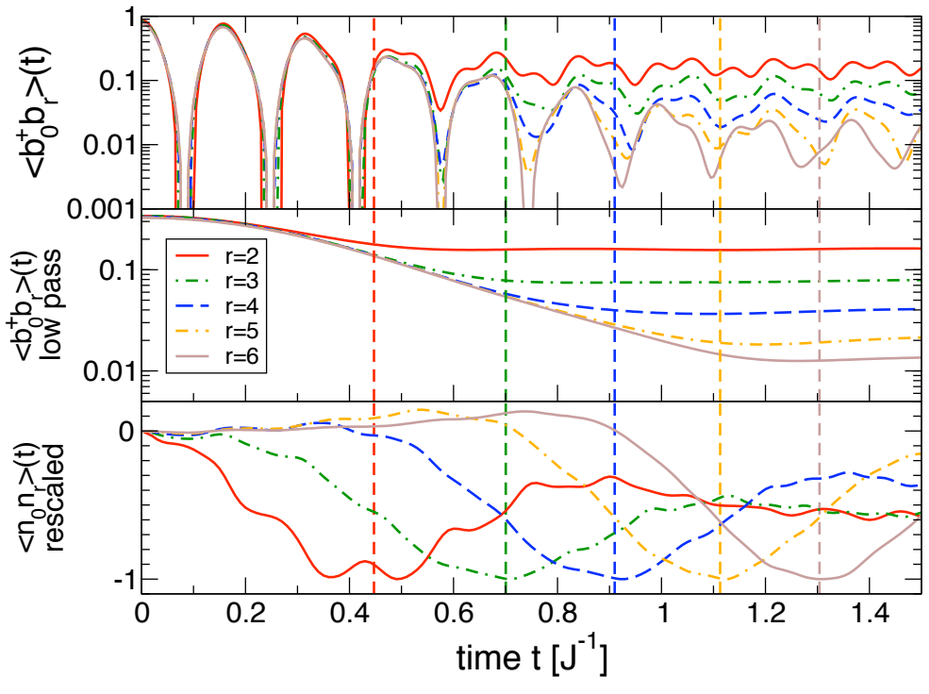
- Time evolution $|\psi(t)\rangle = \exp[-iHt]|\psi(0)\rangle$

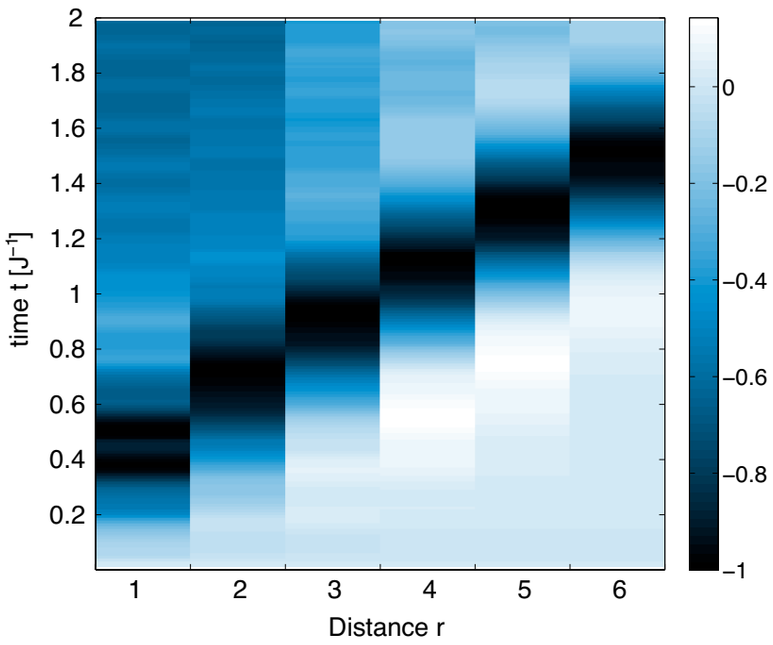
  typically $H = H_0 + H_1\Theta(t), \quad |\psi(0)\rangle = |\psi_0\rangle \text{ or } A^\dagger|\psi_0\rangle$.

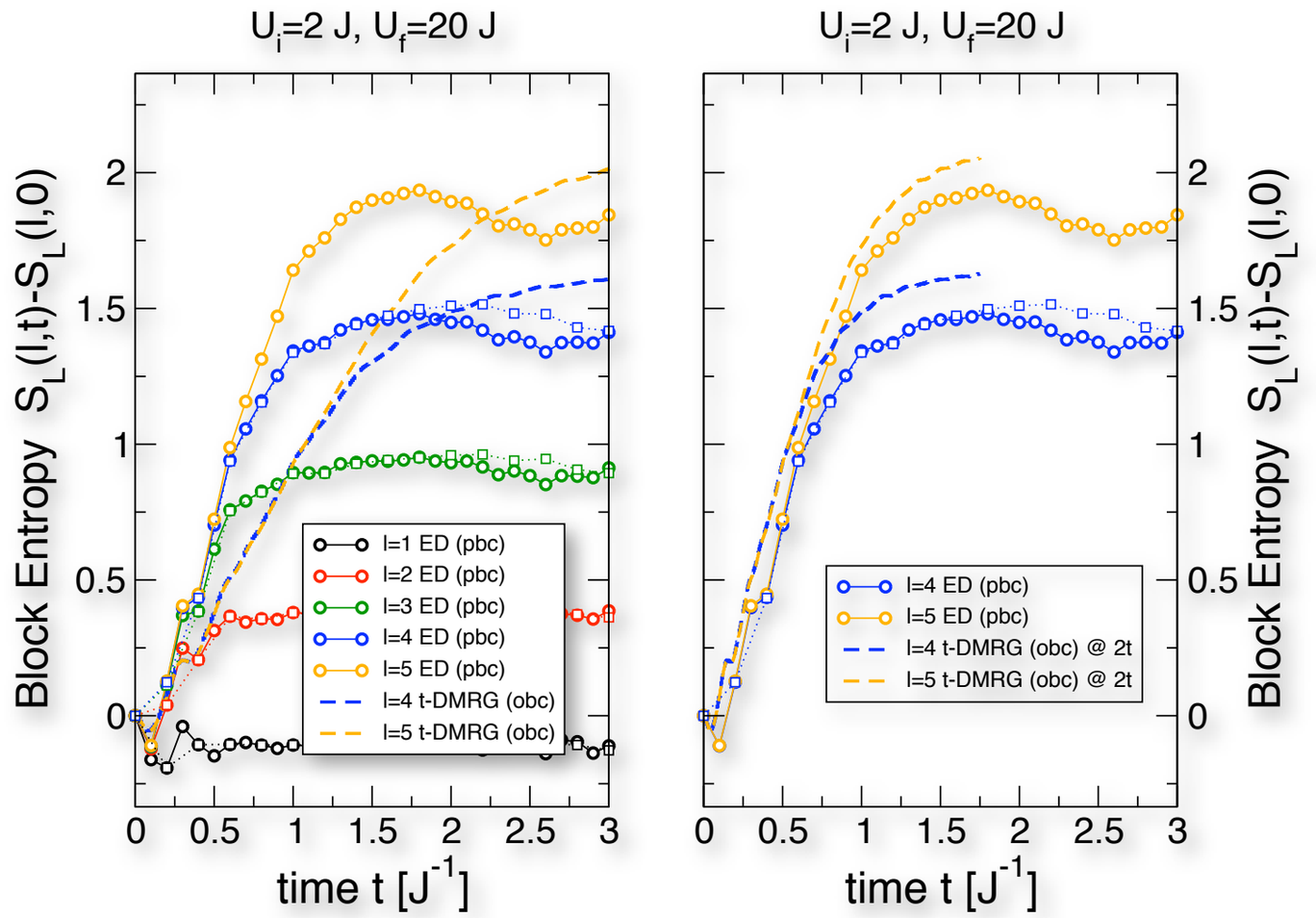
- DMRG Approaches to time evolution
  - Runge Kutta integration of $|\psi_0\rangle_{\mathrm{DMRG}}$ (Cazallila & Marston 2002) only good at small times due to static Hilbert space
  - Division of exp[-iHt] into two site parts which are exactly applied (Vidal; White et al; Daley et al 2003/4) Suzuki-Trotter decomposition, quantum gates.
  - Expansion of exp[-iHt] in Krylov Basis (Schmitteckert; Manmana et al, 2004) multi-target method
- Applications: Tunnel current between Luttinger liquids
  Transport current in a quantum dot
  Quench dynamics
  Dynamical correlation functions (Fourier transform)

Application of t-DMRG
Quench in the Bose Hubbard model

- Start with 1D superfluid initial state, then quench to large U/J value !







AML & Kollath, JSTAT 08

Finite Temperature DMRG

- Many ideas

  - Use Boltzmann weights to weight target states in mixed density matrix
    Works only at low T, but that's also the region where finite size effects are important (Moukouri & Caron 1996)

  - Transfer Matrix DMRG (Bursill et al '1996; Wang & Xiang 1997)
    Uses Suzuki-Trotter decomposition to map onto 1+1 classical system
    Perform DMRG on the Suzuki-Trotter lattice for the transfer matrix
    Imaginary time discrete, but directly for infinite system.

  - Purification approach: (e.g. Feiguin & White, 2005)
    Infinite temperature density matrix of a system can be represented as a pure state of enlarged system. Perform imaginary time evolution to lower temperature T and measure desired quantities (also real-time simulations).

More extensions

- Classical transfer matrices (2D stat mech problem)
- Non-equilibrium classical systems (reaction-diffusion)
- Momentum space DMRG (accurate at small U/t)
- Quantum chemistry
- ...

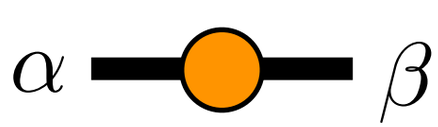
Beyond DMRG

Tensor Networks

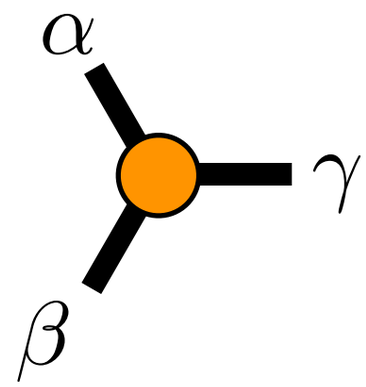
- A nice graphical way to represent tensors and their contractions

Vector

Matrix



rank 3 tensor



Tensor Networks

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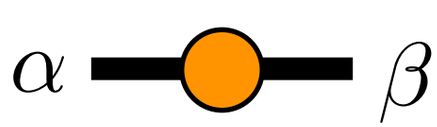
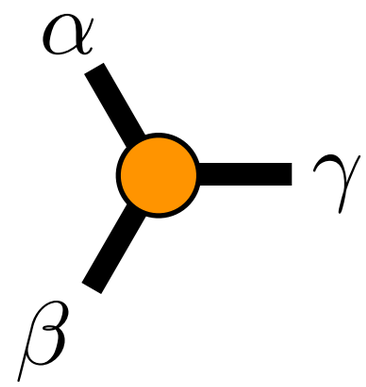
Vector

Matrix



rank 3 tensor

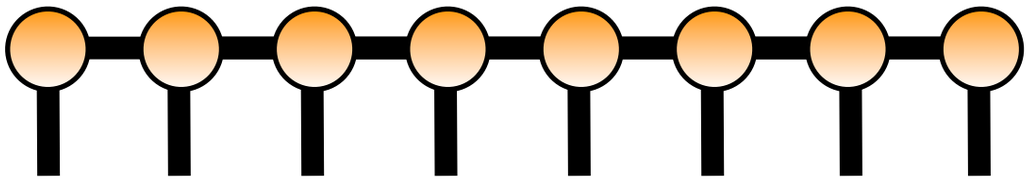


$$Q_{\alpha,\gamma} = (RS)_{\alpha,\gamma} = \sum_{\beta} R_{\alpha,\beta} Q_{\beta,\gamma}$$

Tensor Networks as wave functions

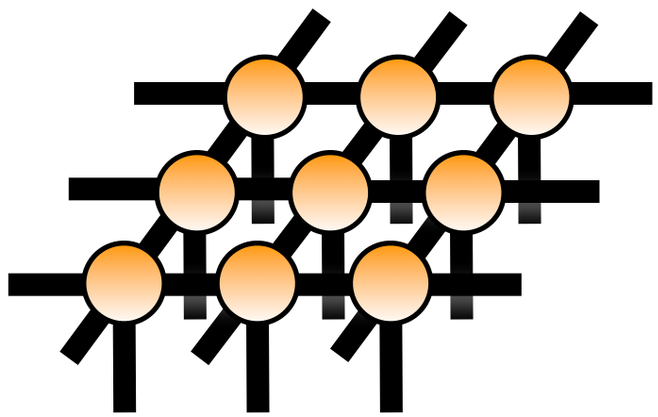
- Matrix Product State (MPS)

$$A[\sigma]_{\alpha,\beta}$$



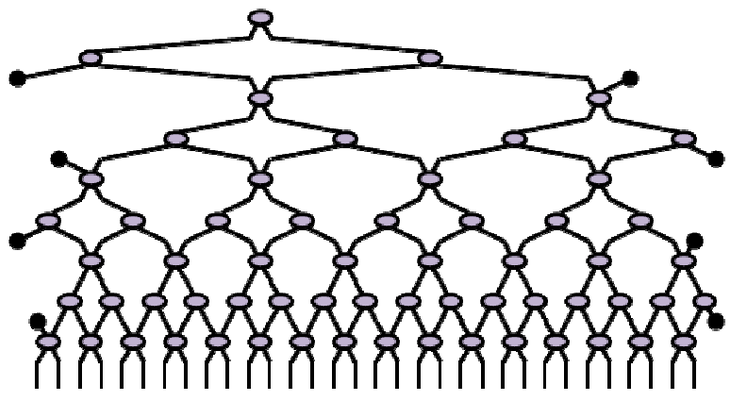
Can satisfy
1D Area laws

- Tensor Product States (TPS), Projected Entangled Pair States (PEPS) (Verstraete & Cirac)



Can satisfy
2D Area laws

- Multiscale Entanglement Renormalization Ansatz (MERA) (Vidal)



Can satisfy
2D Area laws

Tensor Networks as wave functions

- Instead of exponential number of coefficients in the wave functions only O(N d χ^p) coefficients are needed (p=2 for MPS, p=4 for PEPS)

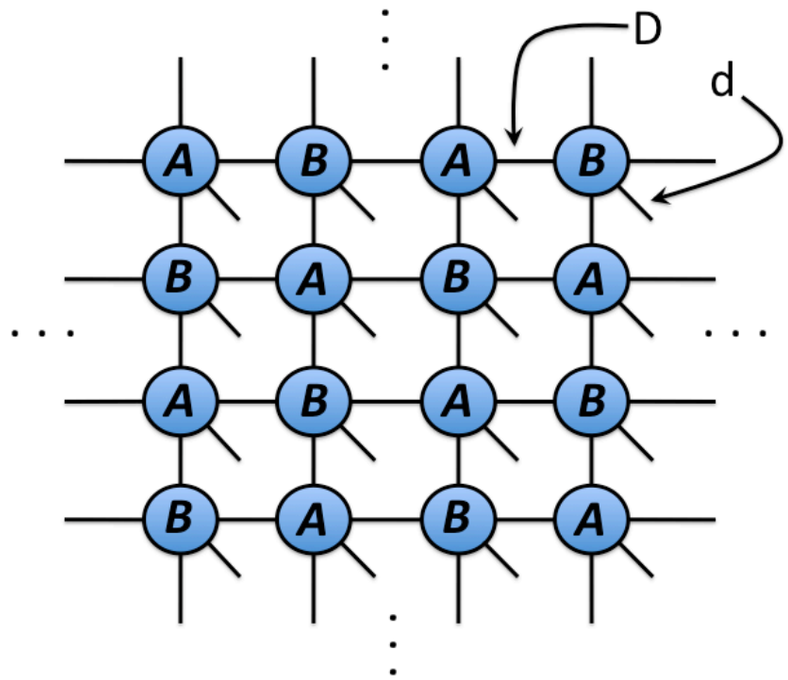
- These tensor networks can be seen as variational wave functions

- The proposed algorithms (PEPS, MERA, ...) contain recipes on how to optimize the network to give the lowest energy for a chosen Hamiltonian

- Not all networks are equally easy to handle.

i-TEBD / i-PEPS

- Assume a translationally invariant ansatz with two matrices in the case of MPS (i-TEBD) or two different tensors in the case of PEPS (i-PEPS)



- Perform imaginary time evolution in order to anneal to the ground state

- i-TEBD is already quite popular as an alternative to DMRG in 1D, and is simple to implement (I saw a Matlab code with 71 lines for the 1D Q-Ising model)

First (finite size) PEPS Applications

- PEPS: Frustrated J_1-J_2-J_3 Square lattice (Murg et al., arXiv:0901.2019)
- Square lattices with open boundary conditions

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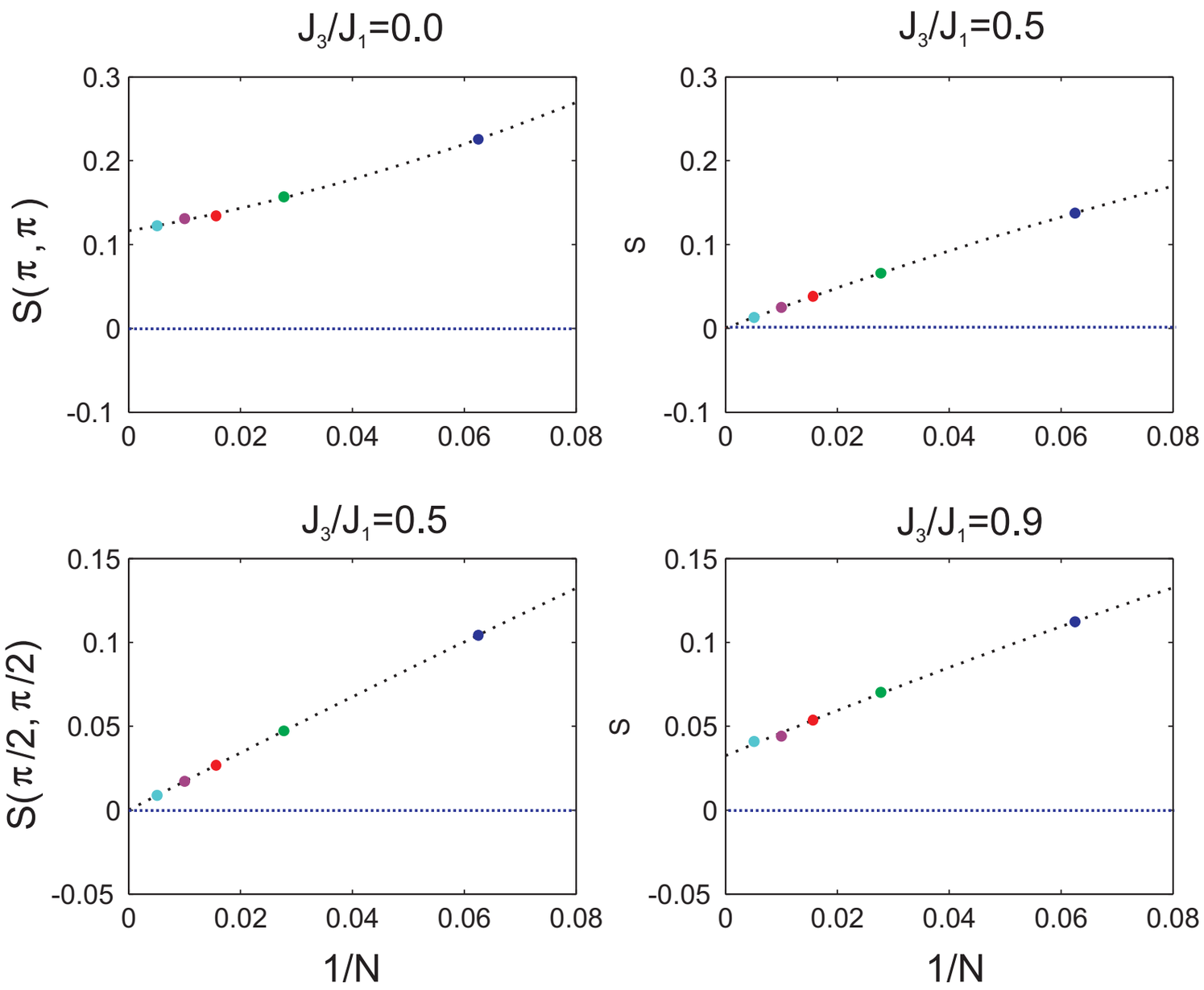

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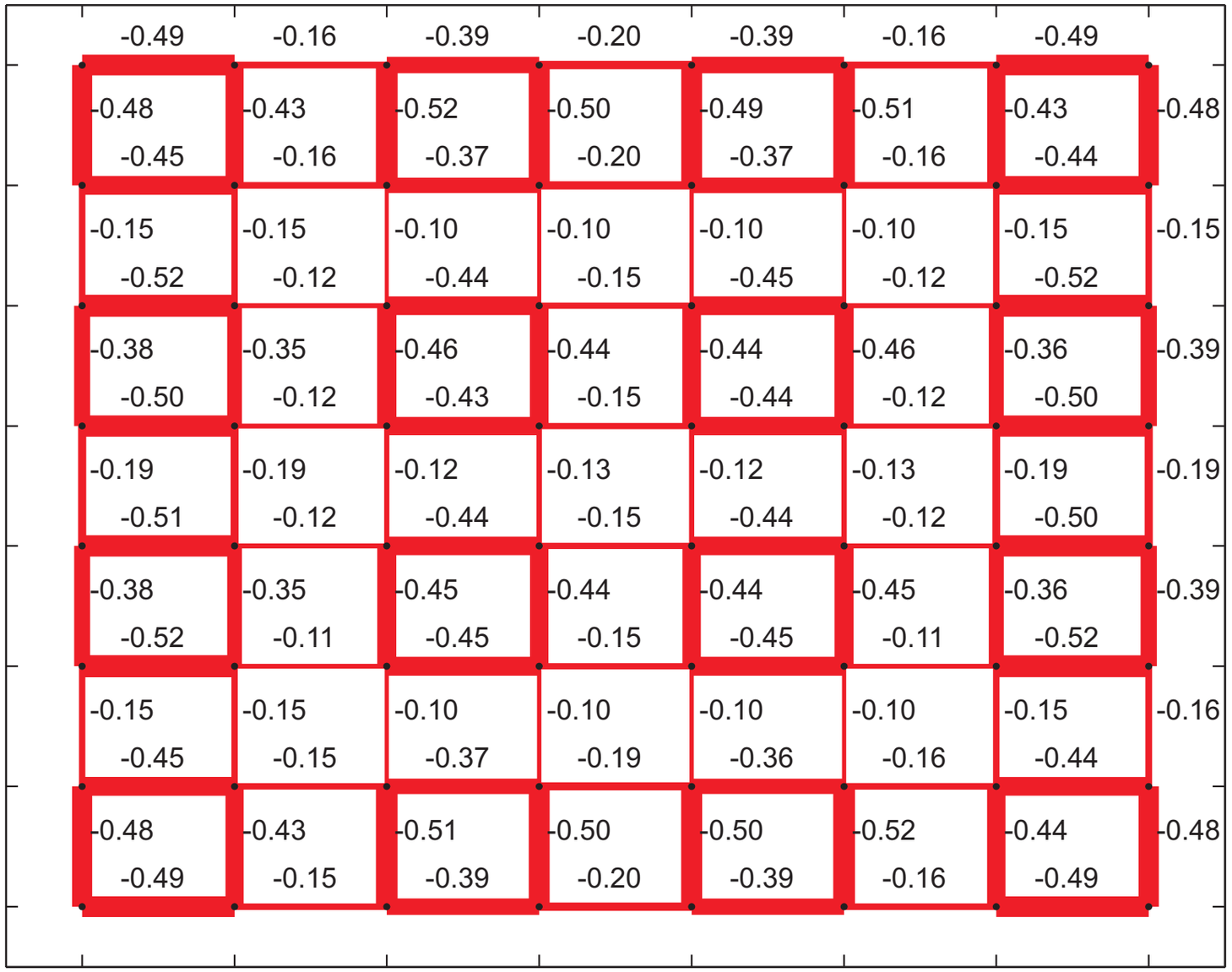
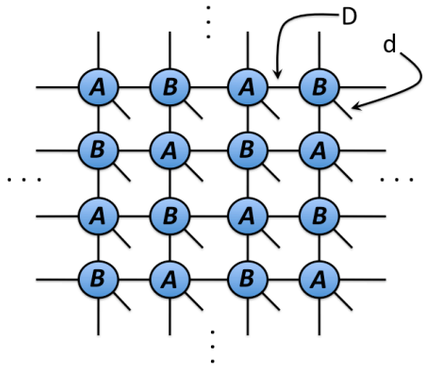
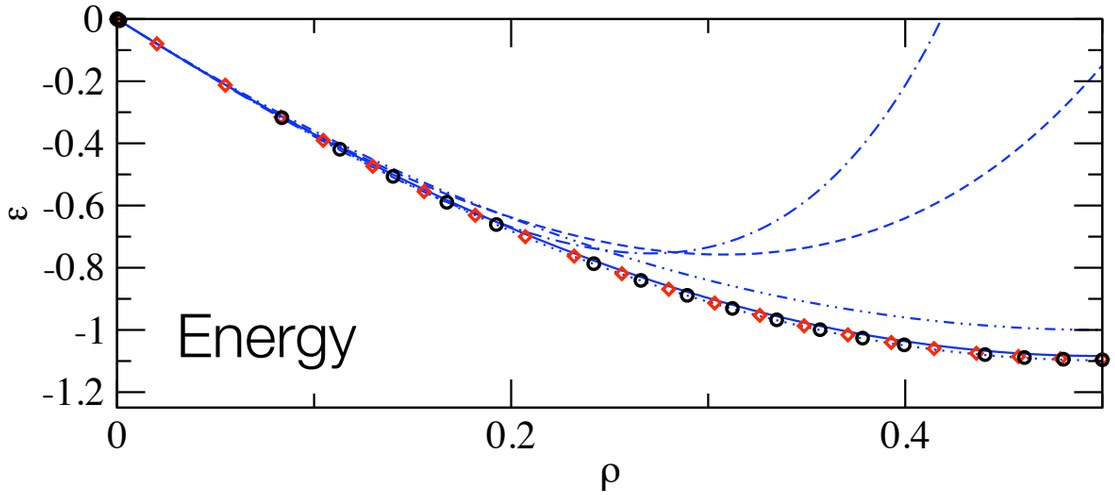
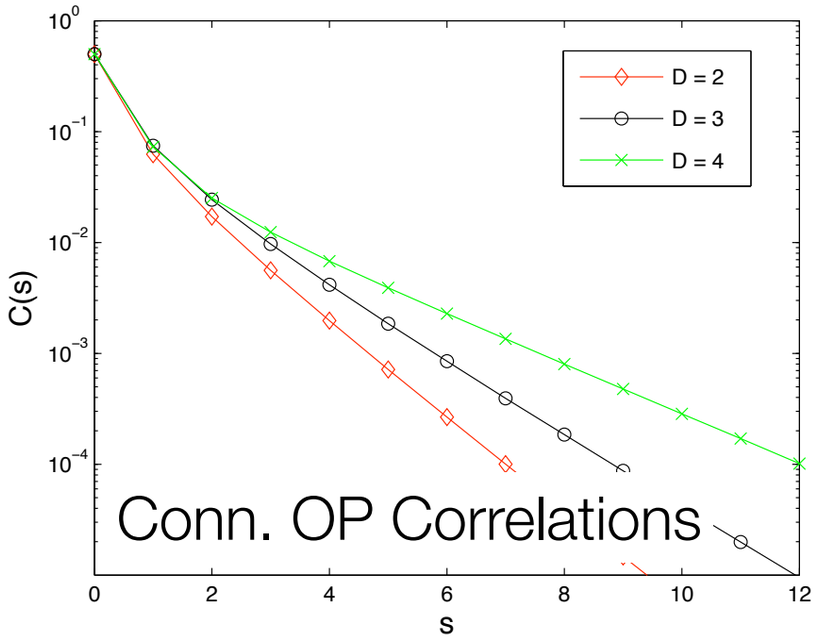


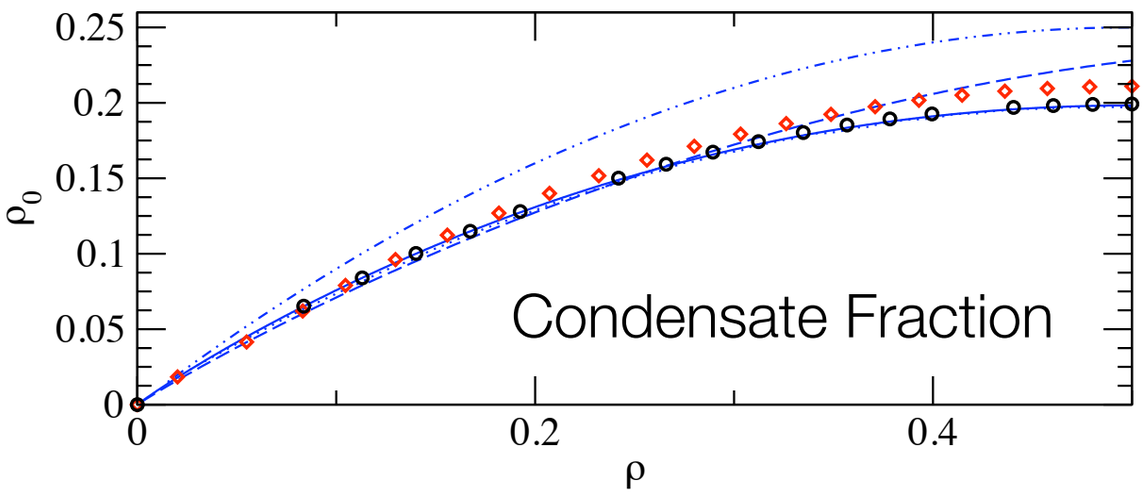
First i-PEPS Applications

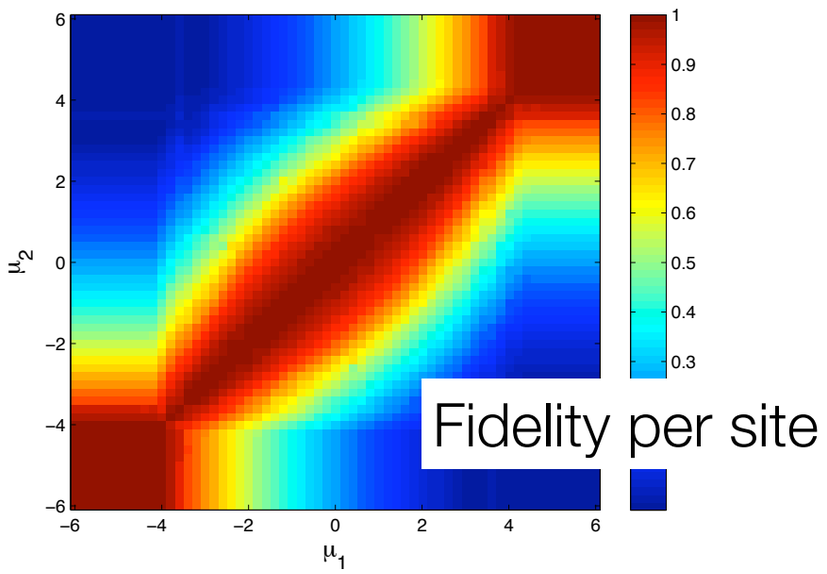


- iPEPS: Hardcore bosons on the square lattice (Jordan et al., arXiv:0901.0420) equivalent to S=1/2 XY model



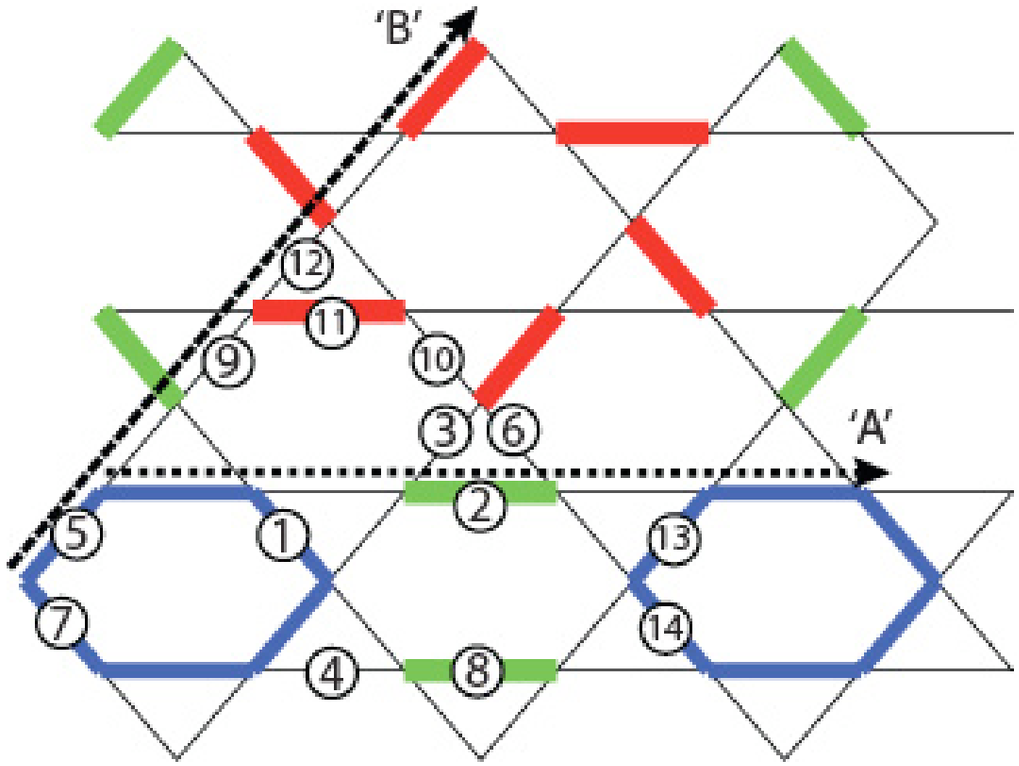


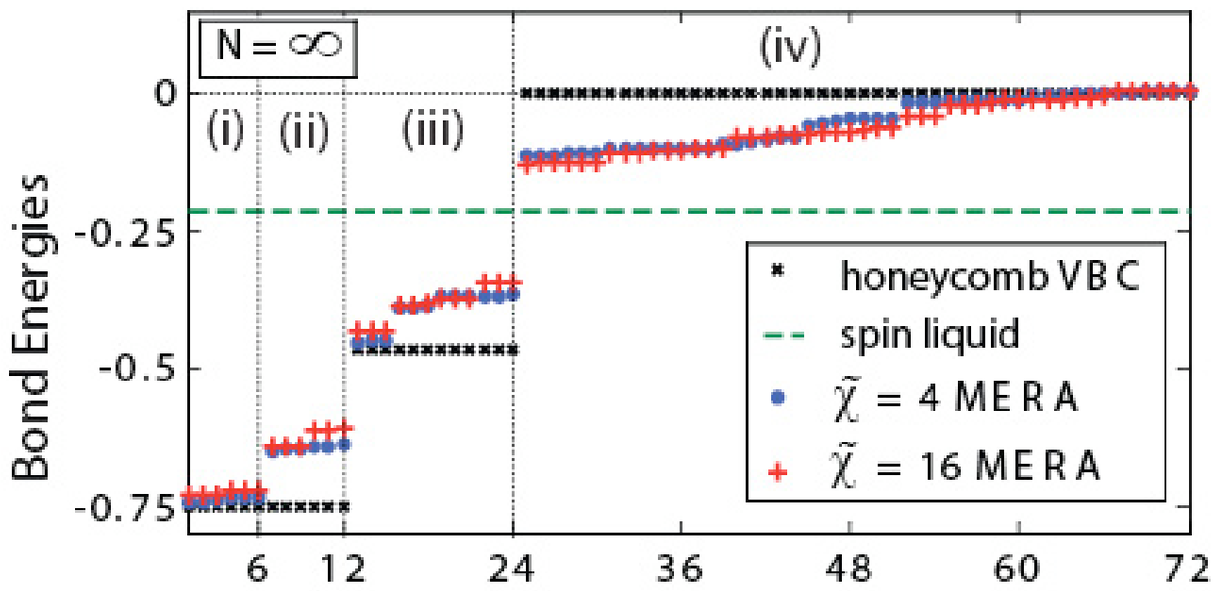




First MERA Applications

- MERA: Kagome lattice Heisenberg model (Evenbly and Vidal, arXiv:0904.3383)
- Confirms the hypothesis of a 36 sites VBC on the kagome lattice





Conclusion

- DMRG is a highly successful method to treat 1D quantum mechanical many body systems at T=0, based on density matrix driven truncation.

- Many extension have been put forward which allow to calculate spectral functions, real time evolution, classical systems in 2D, finite temperature properties, dissipation, ...

- Quantum information theory provided deep insights in the possibilities and limitations of DMRG and proposes new setups to extend DMRG to 2D. However the efficiency of 1D DMRG has not yet been achieved in 2D.

DMRG Literature

- Original papers:

  S.R. White, "*Density matrix formulation for quantum renormalization groups*", Phys. Rev. Lett. **69**, 2863 (1992).

  S.R. White, "*Density-matrix algorithms for quantum renormalization groups*", Phys. Rev. B **48**, 10345 (1993).

- U. Schollwöck, "*The density-matrix renormalization group*", Rev. Mod. Phys. **77**, 259 (2005).

- K. Hallberg, "*New Trends in Density Matrix Renormalization*" Adv. Phys. **55**, 477 (2006).

- R.M. Noack & S. Manmana, "*Diagonalization- and Numerical Renormalization-Group-Based Methods for Interacting Quantum Systems*", AIP Conf. Proc. **789**, 93 (2005).

Thank you !