

Generalized tensor methods and entanglement measurements for models with long-range interactions

Örs Legeza

in collaboration with

- ▶ Jenő Sólyom, Gergely Barcza (Budapest)
- ▶ Florian Gebhard, Reinhard M. Noack (Marburg)
- ▶ Valentin Murg, Frank Verstraete (Wien)
- ▶ Markus Reiher, Konrad H. Marti, Katharina Boguslawski, Pawel Tecmer, Stefan Knecht (Zürich)
- ▶ Thorsten Röhwedder and Reinhold Schneider (Berlin)

Wigner Research Centre for Physics, Budapest

Numerical methods for high-dimensional problems, Paris, 14.04.2014.

Brief historical overview

- ▶ Renormalization Group (Kadanoff transformation) (1966)
- ▶ Block Renormalization Group (BRG) method
- ▶ Numerical Renormalization Group (NRG): Wilson(1975)
- ▶ Density Matrix Renormalization Group (DMRG): White(1992)
- ▶ Quantum chemistry version of DMRG (QC-DMRG):
White(1999),Mitrushenkov(2001),Chan(2002),Legeza(2002),
Reiher(2005),Zgid(2006),Yanai(2008),Xiang(2010),
Ma(2012), Wouters(2013)...
- ▶ Matrix Product State (MPS):
Östlund, Rommer(1995), Cirac, Verstraete(2004),
Oseledets(2009)

Some useful reviews, also see additional references therein

- ▶ U. Schollwöck, *Rev. Mod. Phys.* **77**, 259 (2005).
- ▶ R. M. Noack and S. R. Manmana, in *Diagonalization- and Numerical Renormalization-Group-Based Methods for Interacting Quantum Systems*, (AIP, 2005), vol. 789, pp. 93–163.
- ▶ F. Verstraete, J.I. Cirac, V. Murg, *Adv. Phys.* **57** (2), 143 (2008).
- ▶ Ö. Legeza, R. Noack, J. Sólyom, and L. Tincani, in *Computational Many-Particle Physics*, eds. H. Fehske, R. Schneider, and A. Weisse **739**, 653–664 (2008).
- ▶ U. Schollwöck, *Ann. Phys. (NY)* **326**, 96 (2011).
- ▶ G. K.-L. Chan and S. Sharma, *Annu. Rev. Phys. Chem.* **62**, 465–481 (2011).
- ▶ K. H. Marti and M. Reiher, *Z. Phys. Chem.* **224**, 583-599 (2010). K. H. Marti, M. Reiher, *Phys. Chem. Chem. Phys.* **13** 6750-6759 (2011).
- ▶ G. K.-L. Chan, *Wiley Inter-disciplinary Reviews: Computational Molecular Science* 2 (6) (2012) 907–920.

Some useful reviews, also see additional references therein

- ▶ Ö. Legeza, T. Röhwedder, R. Schneider, Numerical approaches for high-dimensional PDE's for quantum chemistry, in Encyclopedia of Applied and Computational Mathematics, Editor-in-chief: Engquist, Björn ; Chan, T.; Cook, W.J.; Hairer, E.; Hastad, J.; Iserles, A.; Langtangen, H.P.; Le Bris, C.; Lions, P.L.; Lubich, C.; Majda, A.J.; McLaughlin, J.; Nieminen, R.M.; ODEEN, J.; Souganidis, P.; Tveito, A. (Eds.) Springer 2013 ISBN 978-3-540-70530-7
- ▶ Ö. Legeza, T. Röhwedder, R. Schneider, Sz. Szalay, arxiv:1310.2736 (2013).
- ▶ W. Hackbusch, Tensor Spaces and Numerical Tensor Calculus, SSCM Vol. **42**, Springer, 2012.
- ▶ R. Orus, arXiv:1306.2164.
- ▶ <http://tagung-theoretische-chemie.uni-graz.at/en/past-workshops/workshop-2014/>

Topics to be covered

1. Motivation and former approaches:
 - Model Hamiltonian, i.e., problem to solve
 - Problem in the language of tensor factorization
 - Change of basis and truncation
 - Block Renormalization Group (BRG)
 - Numerical Renormalization Group (NRG)
2. New algorithms in quantum chemistry with polynomial costs:
 - Density matrix renormalization group (DMRG) [White,1992](#)
 - Matrix Product State (MPS) [Ostlund,1995](#); [Verstraete,2004](#)
 - Tensor Network States (TNS) [Marti,2010](#); [Murg,2010](#); [Chan,2013](#)
3. One- and Two-orbital mutual information → **Entanglement**
 - Optimizing the algorithms [Legeza,2003](#); [Rissler,2006](#)
 - Efficient construction of active spaces [Legeza,2003](#)

Remark: We give a technical introduction to low rank tensor factorization and do not intend to present a detailed review of the field. Only some selected topics will be covered due to time constraint.

- ▶ In ab initio calculations M atoms, N_e electrons, Coulomb-interaction with $\hbar = e = m = 1$

$$\mathcal{H} = \sum_{i=1}^{N_e} -\frac{\nabla_i^2}{2} - \sum_{i=1, \alpha=1}^{N_e, M} \frac{Z_\alpha}{|r_i - r_\alpha|} + \frac{1}{2} \sum_{i \neq j=1}^{N_e} \frac{1}{|r_i - r_j|}$$

Hamilton-operator, where Z_α is the charge of nucleus α , and r denotes the positions of the nuclei and electrons.

- ▶ The ground state solution is often approximated in a mean-field manner, where the explicit electron-electron interaction is interchanged by an effective single-particle term. The so called Hartree-Fock (HF) solution of the resulting model often recovers the major part (99 %) of the total energy and provides a good starting point for post-HF computations.
- ▶ The correlation energy can be defined as the difference of the exact and the HF energy. The electron correlation, i.e., the beyond mean-field behavior of the electrons, plays an important role in the quantitative description of the chemical properties.

Hamiltonian of the interacting electron system

- ▶ The system is described by the Hamiltonian, for example,

$$\mathcal{H} = \sum_{ij\sigma} T_{ij\sigma} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{ijkl\sigma\sigma'} V_{ijkl\sigma\sigma'} c_{i\sigma}^\dagger c_{j\sigma'}^\dagger c_{k\sigma'} c_{l\sigma}$$

- ▶ T_{ij} denotes the one-electron integral comprising the kinetic energy of the electrons and the external electric field of the nuclei.
- ▶ V_{ijkl} stands for the two-electron integrals and contains the e-e repulsion operator.

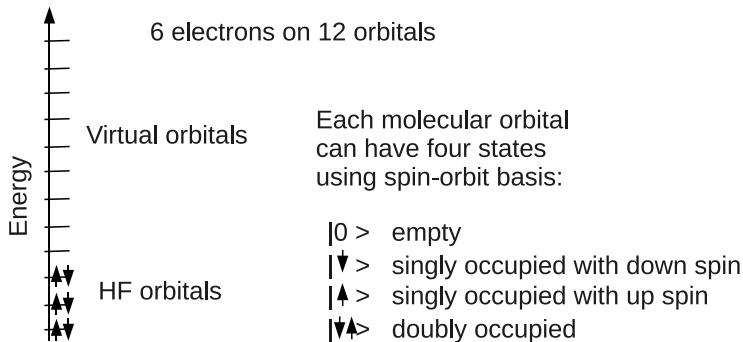
$$V_{ijkl} = \int d^3x_1 d^3x_2 \Phi_i^*(\vec{x}_1) \Phi_j^*(\vec{x}_2) \frac{1}{|\vec{x}_1 - \vec{x}_2|} \Phi_k(\vec{x}_2) \Phi_l(\vec{x}_1)$$

- ▶ Molecular integrals are calculated via one-electron basis of atom-centered Gaussians
- ▶ Major aim: to obtain the desired eigenstates of \mathcal{H} .

Molecular orbitals, configuration space

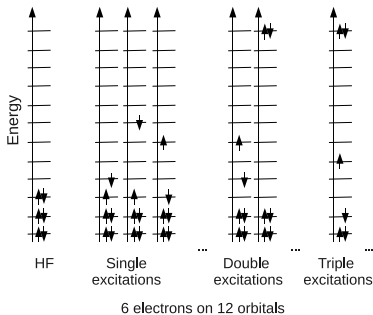
Molecular orbitals are obtained, e.g., in a suitable mean-field or MCSCF calculation (for example using the MOLPRO program package).

Example.: LiF (6/12)



- ▶ Two major approximations:
 - (1) selection of the finite number of basis states
 - (2) restricted number of configurations is taken into account

Corrections to the Hartree-Fock state



- ▶ The full configuration interaction (full-CI) wavefunction can be expressed in terms of Slater determinants by removing one (S), two (D), three (T) or four (Q) electrons from the HF orb.:

$$\Psi_{\text{FCI}} = a_0 \Phi_{\text{SCF}} + \sum_S a_S \Phi_S + \sum_D a_D \Phi_D + \sum_T a_T \Phi_T + \dots$$

- ▶ Correlation energy: $E_{\text{Corr}} = E_{\text{FCI}} - E_{\text{HF}}$.
- ▶ Other expansions are also possible, e.g., Coupled Cluster (see Schneider's talk).

The problem in the language of tensor factorization

- ▶ Local tensor space Λ , with $\dim\Lambda = q$, is denoted by \bullet
- ▶ Operators for basis $|n, \sigma\rangle$ with $n = \{0, 1\}$ and $\sigma = \{\downarrow, \uparrow\}$

$$c^\dagger = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad l_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad Ph_2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- ▶ In a \mathbb{C}^4 representation \bullet represents a spin-orbital basis with $q = 4$. Relevant orbital operators in the $|-\rangle, |\downarrow\rangle, |\uparrow\rangle, |\downarrow\uparrow\rangle$ basis:

$$c_{\downarrow}^\dagger = c^\dagger \otimes l_2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad c_{\uparrow}^\dagger = Ph_2 \otimes c^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$$

$$l = l_2 \otimes l_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad Ph = Ph_2 \otimes Ph_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

The problem in the language of tensor factorization

- ▶ We can put together two \mathbb{C}^4 tensor spaces, i.e., form a two-orbital system ($\bullet\bullet$)
- ▶ $\Lambda^{(1,2)} = \Lambda^{(1)} \otimes \Lambda^{(2)}$ with $\dim\Lambda^{(1,2)} = \dim\Lambda^{(1)}\dim\Lambda^{(2)} = q^2$
- ▶ Basis of the $\bullet\bullet$ system: $|\phi_{\{\alpha_1, \alpha_2\}}^{(1,2)}\rangle = |\phi_{\alpha_1}^{(1)}\rangle \otimes |\phi_{\alpha_2}^{(2)}\rangle$

$$\{\alpha_1, \alpha_2\} = (\alpha_1 - 1)q + \alpha_2 \quad \left| \begin{array}{cc} - & - \\ - & \downarrow \\ - & \uparrow \\ - & \downarrow\uparrow \\ \downarrow & - \\ \downarrow & \downarrow \\ \vdots & \vdots \\ \downarrow\uparrow & \downarrow\uparrow \end{array} \right|$$

$$\alpha_1, \alpha_2 \in \{1, 2, 3, 4\} = \{|\rightarrow\rangle, |\downarrow\rangle, |\uparrow\rangle, |\downarrow\uparrow\rangle\}$$

$$\{\alpha_1\alpha_2\} \in \{1, 2, 3, 4 \dots 16\}$$

The problem in the language of tensor factorization

- ▶ Relevant operators for the $\bullet\bullet$ system ($\dim\Lambda^{(1,2)} = 4 \times 4$):

$$c_{1,\downarrow}^\dagger = c_\downarrow^\dagger \otimes I, \quad c_{2,\downarrow}^\dagger = Ph \otimes c_\downarrow^\dagger, \quad I \Leftarrow I \otimes I,$$

$$c_{1,\uparrow}^\dagger = c_\uparrow^\dagger \otimes I, \quad c_{2,\uparrow}^\dagger = Ph \otimes c_\uparrow^\dagger, \quad Ph \Leftarrow Ph \otimes Ph,$$

$$\mathcal{H} = \begin{pmatrix} h_{1,1} & \dots & h_{1,16} \\ \vdots & \dots & \vdots \\ h_{16,1} & \dots & h_{16,16} \end{pmatrix}$$

- ▶ Full diagonalization of \mathcal{H} gives exact solution (full-CI).
- ▶ The k^{th} eigenstate of a two-orbital Hamiltonian is

$$\Psi_k^{(1,2)} = \sum_{\alpha_1, \alpha_2} U_{\alpha_1, \alpha_2, k}^{(1,2)} |\phi_{\alpha_1}^{(1)}\rangle \otimes |\phi_{\alpha_2}^{(2)}\rangle;$$
$$\alpha_1, \alpha_2 = 1 \dots q; \quad k = 1 \dots q^2.$$

Change of basis and truncation

- ▶ We can represent the Hamiltonian in the eigenbasis of the $\bullet\bullet$ system by a basis state transformation
- ▶ (Order eigenstates in a descending order, and) form an operator from the corresponding eigenstates as:

$$O = \begin{pmatrix} \psi_1^{(1,2)} \\ \psi_2^{(1,2)} \\ \vdots \\ \psi_{q^2}^{(1,2)} \end{pmatrix}, \quad OO^\dagger = \mathbb{I}$$

- ▶ Transform operators to the new basis as $\mathcal{H} \Rightarrow O\mathcal{H}O^\dagger$

$$c_{1,\downarrow}^\dagger \Rightarrow Oc_{1,\downarrow}^\dagger O^\dagger, \quad c_{2,\downarrow}^\dagger \Rightarrow Oc_{2,\downarrow}^\dagger O^\dagger, \quad \text{etc}$$

- ▶ Idea of truncation: select $M < q^2$ states only so $OO^\dagger \neq \mathbb{I}$.

Example: two half-spins on $\bullet\bullet$, $|\phi_{\downarrow}\rangle \equiv |\downarrow\rangle$, $|\phi_{\uparrow}\rangle \equiv |\uparrow\rangle$

$$\Psi_m = \sum_{\alpha_1, \alpha_2} O_{m, 2(\alpha_1 - 1) + \alpha_2} |\phi_{\alpha_1}\rangle \otimes |\phi_{\alpha_2}\rangle, \quad \alpha_1, \alpha_2 \in \{1, 2\} \equiv \{\downarrow, \uparrow\}$$

O	$\downarrow\downarrow$	$\downarrow\uparrow$	$\uparrow\downarrow$	$\uparrow\uparrow$	S^z	S
Ψ_1	1	0	0	0	-1	1
Ψ_2	0	$1/\sqrt{2}$	$1/\sqrt{2}$	0	0	1
Ψ_3	0	$1/\sqrt{2}$	$-1/\sqrt{2}$	0	0	0
Ψ_4	0	0	0	1	1	1

Take column 1 and 3 for \downarrow

Take column 2 and 4 for \uparrow

$$\begin{pmatrix} 1 & 0 \\ 0 & 1/\sqrt{2} \\ 0 & -1/\sqrt{2} \\ 0 & 0 \end{pmatrix} = (B^{(2)}[\downarrow])_{m, \alpha_1}$$

$$\begin{pmatrix} 0 & 0 \\ 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 0 \\ 0 & 1 \end{pmatrix} = (B^{(2)}[\uparrow])_{m, \alpha_1}$$

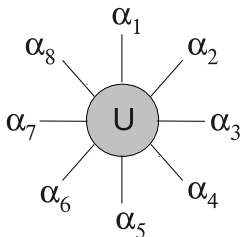
In the literature $A \equiv B^T$ is used.

$$\Psi_m = \sum (A^{(2)}[\alpha_2])_{\alpha_1, m} |\phi_{\alpha_1}\rangle \otimes |\phi_{\alpha_2}\rangle$$

The problem in the language of tensor factorization

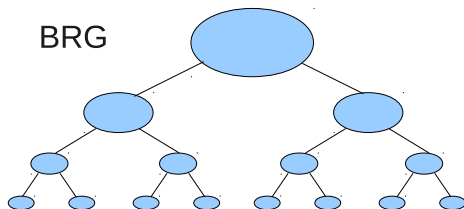
- ▶ For a system with N molecular orbitals: ●●●...●
- ▶ $\Lambda^{(1,2,\dots,N)} = \otimes_{i=1}^N \Lambda^{(i)}$ with $\dim \Lambda^{(1,2,\dots,N)} = \prod_i^N \dim \Lambda^{(i)} = q^N$
- ▶ $\Psi_k^{(1,2,\dots,N)} = \sum_{\alpha_1 \dots \alpha_N} U_{\alpha_1, \alpha_2, \dots, \alpha_N, k}^{(1,2,\dots,N)} |\phi_{\alpha_1}^{(1)}\rangle \otimes |\phi_{\alpha_2}^{(2)}\rangle \otimes \dots \otimes |\phi_{\alpha_N}^{(N)}\rangle$;
- ▶ $U_{\alpha_1, \alpha_2, \dots, \alpha_N, k}^{(1,2,\dots,N)}$ is a tensor of order N corresponding to the k^{th} eigenstate of the N -orbital Hamiltonian

Example: $N = 8$



- ▶ Problem: dimension of U scales exponentially with N
→ We need approximative methods

Idea of renormalization: Block Hamiltonians



- First we form two-orbital Hamiltonians (blocks) from every two-orbitals and diagonalize them to obtain their eigenstates:

$$\Psi_k^{(1,2)} = \sum_{\alpha_1, \alpha_2} U_{\alpha_1, \alpha_2, k}^{(1,2)} |\phi_{\alpha_1}^{(1)}\rangle \otimes |\phi_{\alpha_2}^{(2)}\rangle$$

$$\Psi_k^{(3,4)} = \sum_{\alpha_3, \alpha_4} U_{\alpha_3, \alpha_4, k}^{(3,4)} |\phi_{\alpha_3}^{(3)}\rangle \otimes |\phi_{\alpha_4}^{(4)}\rangle$$

$$\Psi_k^{(5,6)} = \sum_{\alpha_5, \alpha_6} U_{\alpha_5, \alpha_6, k}^{(5,6)} |\phi_{\alpha_5}^{(5)}\rangle \otimes |\phi_{\alpha_6}^{(6)}\rangle$$

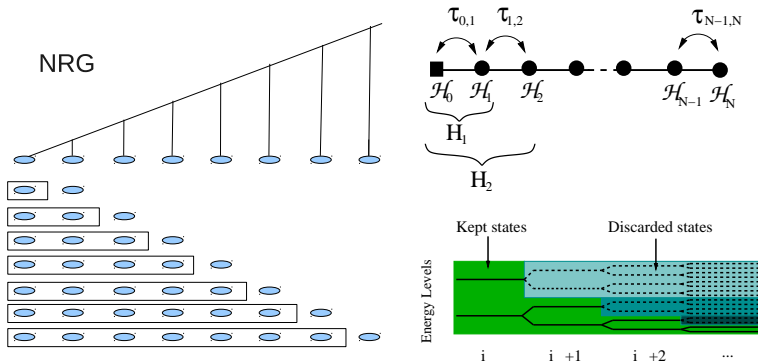
$$\Psi_k^{(7,8)} = \sum_{\alpha_7, \alpha_8} U_{\alpha_7, \alpha_8, k}^{(7,8)} |\phi_{\alpha_7}^{(7)}\rangle \otimes |\phi_{\alpha_8}^{(8)}\rangle$$

$$\alpha = 1 \dots q \text{ and } k = 1 \dots q^2$$

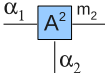
Idea of renormalization: Truncation



- ▶ The original idea was that in each RG step we truncate the Hilbert space of the blocks by keeping only q new states out of the q^2 eigenstates states.
- ▶ The original form of the Hamiltonian is retained, for lattice models analytic solution is possible (flow equations, fixed-point, etc (Example: ITF model))
- ▶ we can keep $q < M \ll q^N$ states but we loose analytic solution, new operators appear (NRG)
- ▶ In general we keep dimension of the Hilbert space under control but we loose information \rightarrow approximate solution of the problem
- ▶ Questions:
 - how to choose which states to keep at each RG step?
 - how many states to keep at each RG step?
 - how accurate will be the truncated solution compared to the full-CI solution?




Numerical Renormalization Group (NRG) method



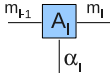
- ▶ With exponentially decreasing hopping amplitude, $t_n = \lambda^{-n/2}$, where λ is the discretization parameter.
- ▶ Lowest lying $q < M \ll q^N$ states are kept at each RG iteration step (works due to separation of energy scales).
- ▶ Problems for lattice models with $\lambda \rightarrow 1$, blocks are formed with open boundary condition, segmentation of the total system

- $|m_2\rangle = \sum_{m_1, \alpha_2} (A^2[\alpha_2])_{\alpha_1; m_2} |\alpha_1\rangle \otimes |\alpha_2\rangle,$ 

- Use the identity: $|m_1\rangle = \sum_{\alpha_1} (A^1[\alpha_1])_{1; m_1} |\alpha_1\rangle,$  

- $|m_3\rangle = \sum_{m_2, \alpha_3} (A^3[\alpha_3])_{m_2; m_3} |m_2\rangle \otimes |\alpha_3\rangle,$   

Transfer tensor:

$$|m_l\rangle = \sum_{m_{l-1}, \alpha_l} (A^l[\alpha_l])_{m_{l-1}; m_l} |m_{l-1}\rangle \otimes |\alpha_l\rangle,$$


Series of transfer tensors:

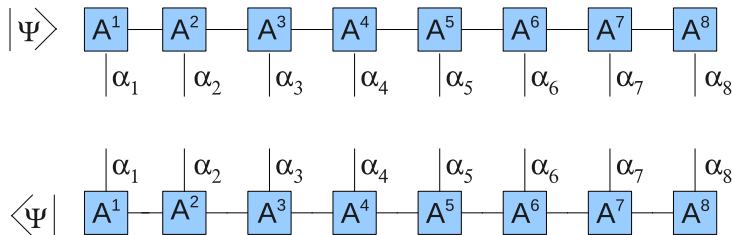
$$|m_l\rangle = \sum_{\alpha_1, \dots, \alpha_l} (A^2[\alpha_2] \dots A^l[\alpha_l])_{\alpha_1; m_l} |\alpha_1 \dots \alpha_l\rangle,$$

For each molecular orbital we can assign a matrix: $(A^l[\alpha_l])_{m_{l-1}; m_l}$ and the wavefunction can be expressed as a product of matrices.

Tensor product approximations:

- ▶ Matrix Product State (MPS) representation:

$$|\Psi\rangle = \sum_{\alpha_1, \alpha_2, \dots, \alpha_N}^q A_{\alpha_1}^1 A_{\alpha_2}^2 \cdots A_{\alpha_N}^N |\alpha_1\rangle |\alpha_2\rangle \cdots |\alpha_N\rangle$$

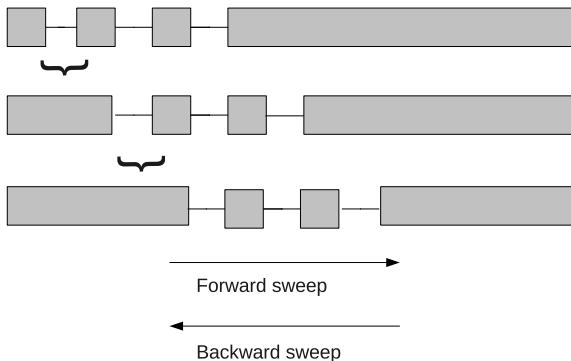


$$A_i[m, m]_{q_i}$$

- ▶ We can call this a network. Matrix product state (MPS) / Tensor Train (TT): Ostlund, Rommer (1995), Verstraete, Cirac (2004), Oseledets (2009), Hackbusch (2009)

DMRG provides MPS wavefunction:

Density matrix renormalization group wavefunction: (White, 1992)



$$|\psi_{\text{TG}}\rangle = \sum_{\alpha_l \alpha_{l+1} \alpha_{l+2} \alpha_r} \psi_{\alpha_l \alpha_{l+1} \alpha_{l+2} \alpha_r} |\phi_{\alpha_l}^{(l)}\rangle \otimes |\phi_{\alpha_{l+1}}^{(s_l)}\rangle \otimes |\phi_{\alpha_{l+2}}^{(s_r)}\rangle \otimes |\phi_{\alpha_r}^{(r)}\rangle$$

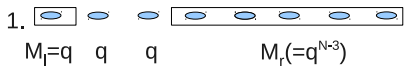
where $\psi_{\alpha_l \alpha_{l+1} \alpha_{l+2} \alpha_r}$ coefficients are determined by an iterative diagonalization of the superblock Hamiltonian.

DMRG algorithm provides the optimized set of A_i matrices.

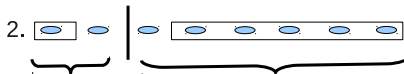
DMRG Superblock configuration ($l+1+1+r=N$)

System block with l orbitals

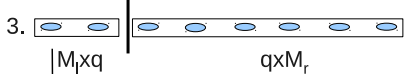
Environment block with r orbitals



Form Hamiltonian and diagonalize



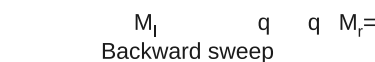
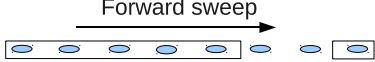
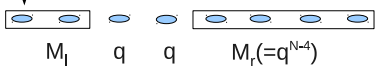
Form bi-partite representation



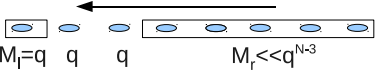
Form system block reduced density matrix

1 DMRG iteration step

4. Diagonalize reduced density matrix
Truncate basis
Renormalize operators

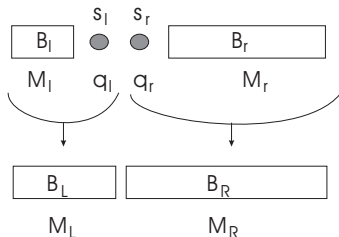


Sweeping



DMRG transforms Single-particle basis states to multi-particle basis states

Similar to non-error free data compression



1. Form and diagonalize the superblock Hamilton operator

$$|\Psi_{\text{TG}}\rangle = \sum_{\alpha_l \alpha_{l+1} \alpha_{l+2} \alpha_r} \psi_{\alpha_l \alpha_{l+1} \alpha_{l+2} \alpha_r} |\phi_{\alpha_l}^{(l)}\rangle \otimes |\phi_{\alpha_{l+1}}^{(s_l)}\rangle \otimes |\phi_{\alpha_{l+2}}^{(s_r)}\rangle \otimes |\phi_{\alpha_r}^{(r)}\rangle$$

where $\psi_{\alpha_l \alpha_{l+1} \alpha_{l+2} \alpha_r}$ coefficients are determined by an iterative diagonalization of the superblock Hamiltonian.

2. Form a bi-partite representation $|\Psi_{\text{TG}}\rangle = \sum_{ij} \psi_{i,j} |\phi_i^{(L)}\rangle |\phi_j^{(R)}\rangle$
3. Form reduced subsystem density matrix $\rho_{i,i'}^{(L)} = \sum_j \psi_{i,j} \psi_{i',j}^*$
4. Diagonalize $\rho \rightarrow \omega_\alpha$ eigenvalues, $|\phi_\alpha^{(L)}\rangle$ eigenstates
5. Form O matrix using M selected $|\phi_\alpha^{(L)}\rangle$ eigenstates corresponding to the M largest ω_α
6. Renormalize operators: $c_i \Rightarrow O c_i O^\dagger$

Schmidt-decomposition for a bipartite system

- ▶ For a bipartite system: $|\Psi_T\rangle = \sum_{ij} \psi_{ij} |\phi_i^L\rangle \otimes |\phi_j^R\rangle$
- ▶ Reduced density matrix: $\rho_{i,i'}^{(L,R)} = \sum_j \psi_{ij} \psi_{i'j}^*$
- ▶ If $|\Psi\rangle$ **pure state** then for $|\Psi\rangle \in \Lambda = \Lambda^L \otimes \Lambda^R$

$$|\Psi\rangle = \sum_{i=1}^{r \leq \min(M_L, M_R)} \omega_i |e_i\rangle \otimes |f_i\rangle.$$

- ▶ $|e_i\rangle, |f_i\rangle$ biorthogonal basis, and r is the Schmidt number
- ▶ If $r = 1 \Rightarrow$ product state, for example, $|\downarrow\uparrow\rangle|\downarrow\uparrow\rangle$
- ▶ If $r > 1 \Rightarrow$ **entangled state: non-local** property of quantum mechanics. Example: $1/\sqrt{2}(|\downarrow\rangle|\uparrow\rangle - |\uparrow\rangle|\downarrow\rangle)$
- ▶ **Neumann entropy**: $s(\rho^\gamma) = -\text{Tr}(\rho^\gamma \ln \rho^\gamma)$, $\gamma \equiv L, R$
- ▶ $|\Psi_T\rangle$ pure state $\rightarrow s(\rho^L) = s(\rho^R)$
- ▶ In general, ρ^L and ρ^R are in **mixed state**

DMRG wavefunction in MPS form for the $l - \bullet \bullet - r$ superblock

$$\begin{aligned}\Psi &= \sum_{\{\alpha\}} \sum_{m^l} \sum_{m^r} \psi_{m^l \alpha_{l+1} \alpha_{l+2} m^r} \\ &\quad \times (B_l[\alpha_l] \dots B_2[\alpha_2])_{m^l; \alpha_1} \\ &\quad \times (B_{l+3}[\alpha_{l+3}] \dots B_{N-1}[\alpha_{N-1}])_{m^r; \alpha_N} \times |\alpha_1 \dots \alpha_N\rangle,\end{aligned}$$

Connection to the CI-type wavefunction (Marti, Reiher 2011)

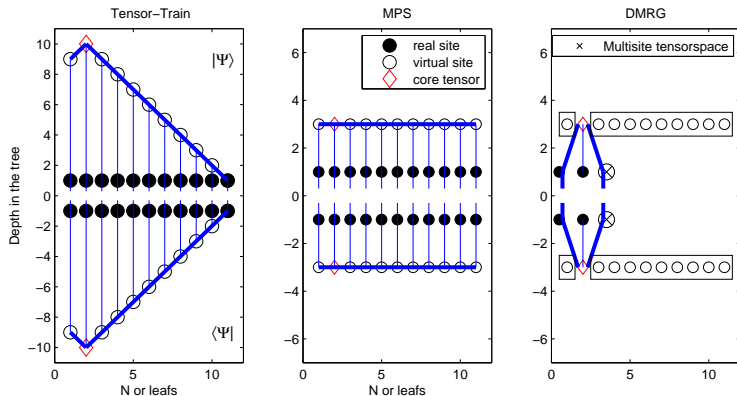
$$\Psi = \sum_{\{\alpha\}} C_{\{\alpha\}} \Phi_{\{\alpha\}},$$

Therefore, the CI-coefficients in MPS form:

$$\begin{aligned}C_{\{\alpha\}} &= \sum_{m^l}^{M_l} \sum_{m^r}^{M_r} \psi_{m^l \alpha_{l+1} \alpha_{l+2} m^r} \\ &\quad \times (B_l[\alpha_l] \dots B_2[\alpha_2])_{m^l; \alpha_1} \times (B_{l+3}[\alpha_{l+3}] \dots B_{N-1}[\alpha_{N-1}])_{m^r; \alpha_N}\end{aligned}$$

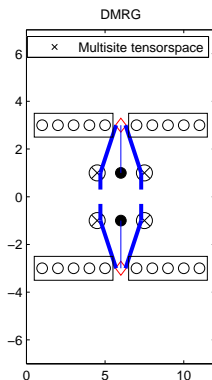
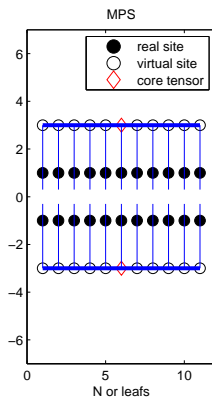
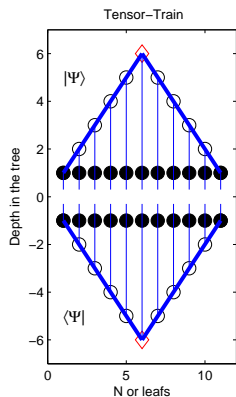
Pictorial/diagrammatic description of the one-site DMRG

- ▶ Component tensors by a dot (or vertex).
- ▶ Each index or variable by a single line coming out of the vertex
- ▶ Line connecting two tensors corresponds to an index over which one has to sum. We call this contraction.
- ▶ DMRG: on the level of operators; MPS: on the level of states.



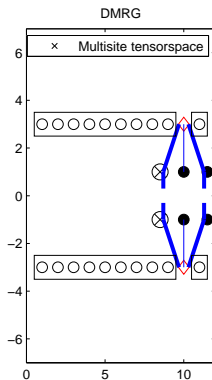
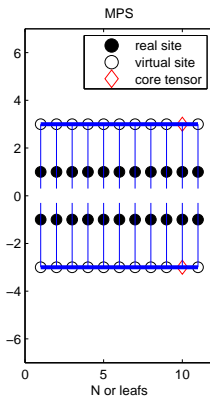
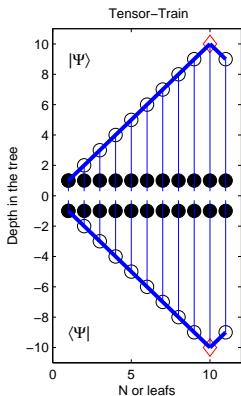
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Pictorial/diagrammatic description of the one-site DMRG

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Error sources and data sparsity

- ▶ In each DMRG step, the basis states of the system block are transformed to a new truncated basis set by a unitary transformation based on the preceding SVD
- ▶ This transformation depends on how accurately the environment is represented and on the level of truncation
- ▶ Environmental error, $\delta\varepsilon_{\text{sweep}}$, is minimized by a successive application of the sweepings
- ▶ Truncation error: $\delta\varepsilon_{\text{TR}} = 1 - \sum_{\alpha=1}^M \omega_{\alpha}$
- ▶ For $\delta\varepsilon_{\text{sweep}} \rightarrow 0$, $\delta E_{\text{rel}} = \text{Const} \times \delta\varepsilon_{\text{TR}}$ (Ö.L. and G. Fáth, PRB 1996).
- ▶ DMRG is a variational method
- ▶ DMRG is a data-sparse representation of the wavefunction

$$\text{sparsity} \equiv \dim(\Lambda_{\text{SB}}) / \dim(\Lambda_{\text{FCI}})$$

Target state

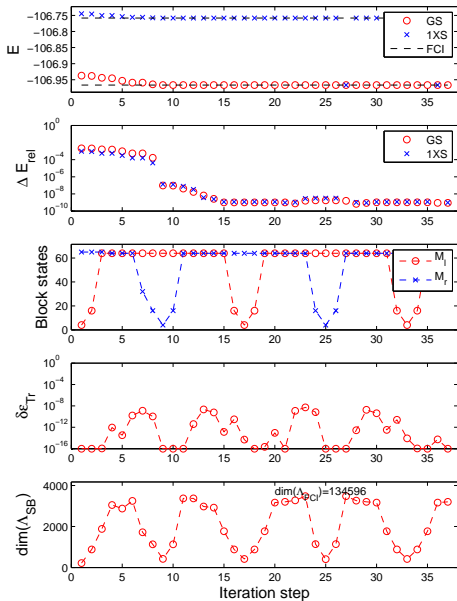
- ▶ In the MPS-based approaches, several eigenstates can be calculated within a single calculation.
- ▶ Reduced density matrix of the target state, ρ , can be formed from the reduced density matrices of the lowest n eigenstates as

$$\rho = \sum_{\gamma} p_{\gamma} \rho_{\gamma}$$

with $\gamma = 1 \dots n$, $\sum_{\gamma} p_{\gamma} = 1$ and $\text{Tr} \rho_{\gamma} = 1$.

- ▶ Excited states corresponding to the action of given operators can also be mixed (see Noack's talk).

Example: targeting several states together



Dynamic Block State Selection (DBSS) procedure

Optimal truncation scheme: $\delta\epsilon_{TR} < \epsilon$ fixed in advance

→ M is chosen accordingly in every step

Example from 2002: DBSS approach applied on F_2 (D_{2h}) (18/18)

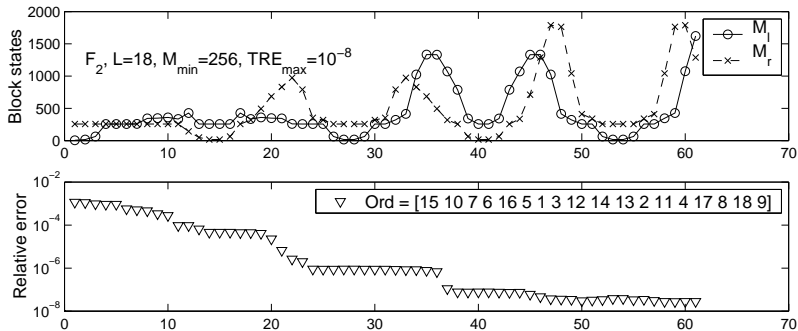
$$\Lambda_{\text{FCI}} = (2N)! / [(2N - N_e)! N_e!] = 9075135300$$

$$\Lambda_{\text{DMRG}} = M_l \times 4 \times 4 \times M_r = 28800000 \quad (M_l = 1200, M_r = 1500)$$

sparsity $\simeq 315$

$$\Lambda_{\text{DMRG}} = M_l \times 4 \times 4 \times M_r = 7680 \quad (M_l = 120, M_r = 4)$$

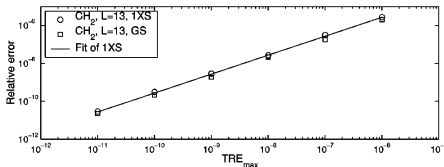
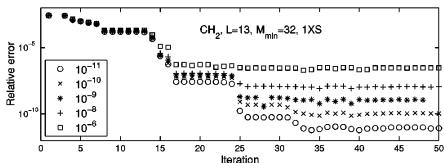
sparsity $\simeq 1181658$ Ö.L. , Roder, Hess, Phys Rev B (2002)



A priori defined error margin for ground and excited states

One can define the required accuracy prior to the calculations

All parameters of the algorithm are adjusted dynamically based on the strength of entanglement encoded in the wavefunction



Part III

Entanglement based optimizations

- ▶ Block entropy → Entanglement
 - Controlling accuracy
 - Controlling convergence
 - Kullback-Leibler relative entropy
- ▶ One- and Two-orbital mutual information → Entanglement
 - Optimizing the algorithms
 - Efficient construction of active spaces
 - Entanglement and change of basis
 - Correlation functions and entanglement
 - Identifying static, dynamic correlations
 - Description of bond formation and breaking procedures

Block entanglement



$$\rho = |\psi\rangle\langle\psi|$$



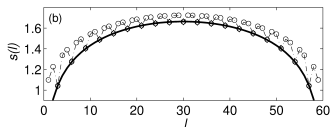
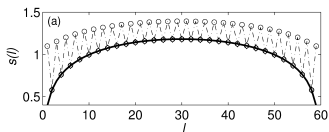
$$\rho^B = \text{Tr}_A \rho$$

$$S^B = -\text{Tr}(\rho^B \ln \rho^B)$$



For critical 1 - d systems : $s_N(l) = \frac{c}{6} \ln \left[\frac{2N}{\pi} \sin \left(\frac{\pi l}{N} \right) \right] + g$,

Vidal, Latorre, Rico, Kitaev, PRL (2005), Calabrese, Cardy, JSM (2004),

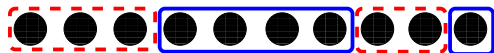


Laflorencie, Sørensen, Chang, Affleck, PRL (2006), Ö.L., Sólyom, Tincani, Noack, PRL (2007)

Mutual information: entanglement correlation



$$\rho = |\psi\rangle\langle\psi|$$

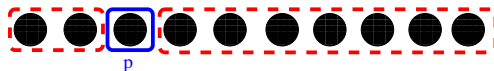


A subsystem

B subsystem

$$\rho^B = \text{Tr}_A \rho$$

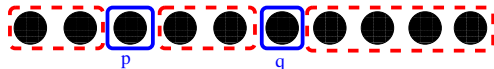
$$S^B = -\text{Tr}(\rho^B \ln \rho^B)$$



p

$$\rho^p \Rightarrow S^p$$

S^p describes the entanglement of site p with the rest of the system.



p

q

$$\rho^{p,q} \Rightarrow S^{p,q}$$

$S^{p,q}$ describes the entanglement of site p and q with the rest of the system.
 $I^{p,q}$ describes the mutual information between site p and q

$$I^{p,q} = (S^p + S^q - S^{p,q})(1 - \delta_{p,q})$$

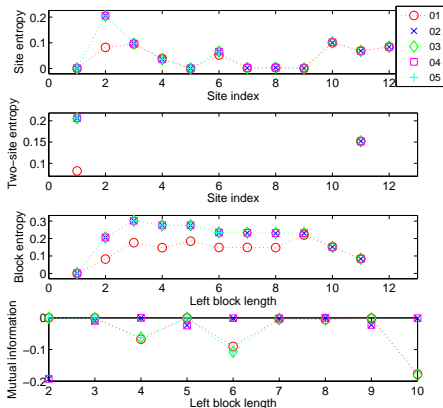
Ö.L., Sólyom, PRB (2003): Quantum Chemistry,

Ö.L., Sólyom, PRL (2005): quantum phase transitions (QPT) with $q = p + 1$.

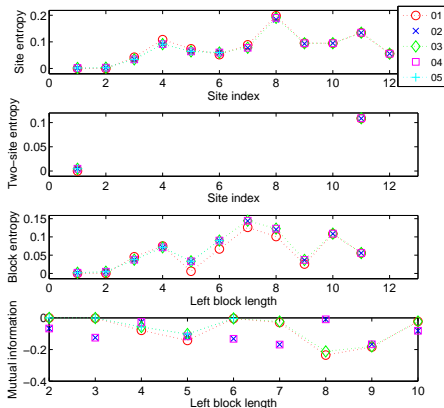
Rissler, White, Noack, ECP (2005): Quantum chemistry, arbitrary p and q .

Block entropy profiles in quantum chemistry (LiF 6/12)

Non-optimized tensor topology



Optimized tensor topology



- Results as a function of sweepings indicated by different colors
- Mutual information: entropy reduction by forming enlarged blocks:

Dynamic Block State Selection (DBSS) procedure

- ▶ To control the weight of retained information during the RG procedure:

$$\rho^{(L)} = p_{\text{kept}} \rho_{\text{kept}}^{(L)} + (1 - p_{\text{kept}}) \rho_{\text{lost}}^{(L)},$$

where $\rho_{\text{kept}}^{(L)}$ is formed from the M largest eigenvalues of $\rho^{(L)}$ and $\rho_{\text{lost}}^{(L)}$ from the remaining eigenvalues with $\text{Tr} \rho_{\text{kept}}^{(L)} = \text{Tr} \rho_{\text{lost}}^{(L)} = 1$.

- ▶ The accessible information for such a binary channel would be less than the Kholevo bound

$$\chi \leq S(\rho) - p_{\text{kept}} S(\rho_{\text{kept}}) - (1 - p_{\text{kept}}) S(\rho_{\text{lost}}),$$

- ▶ In DMRG the atypical subspace is neglected \rightarrow loss of information.
- ▶ **truncation scheme:** $\chi \equiv S(\rho) - S(\rho_{\text{kept}}) < \epsilon$ fixed in advance $\rightarrow M$ is chosen accordingly in every step.

- ▶ Entropy reduction by forming an enlarged system:

$$s_L(l) + s_{l+1} + I_L(l) = s_L(l+1), \quad \text{with} \quad I_L(l) \leq 0$$

- ▶ Obtained correlation in one RG step:

$$I_L(l) = s_L(l+1) - s_L(l) - s_{l+1} \quad 1 \leq l < N-1$$

- ▶ Entropy sum rule:

$$\sum_{l=1}^{N-1} I_L(l) = -\sum_{l=1}^N s_l.$$

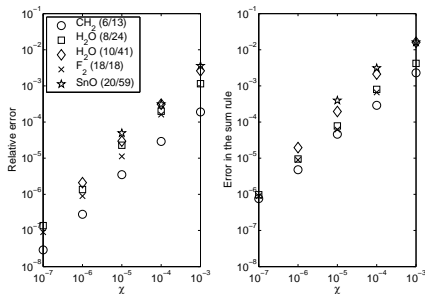
- ▶ In case of truncation:

$$\sum_{l=1}^{N-1} I_L(l) + \sum_{l=1}^N s_l < (N-1)\epsilon$$

a. Real system



b. Real system



- ▶ For $L = N - 2 \rightarrow r = M_L = M_R = 1$, correlation functions

Effect of the environment block \rightarrow efficient warmup

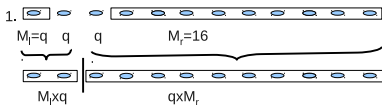
- ▶ New block states after SVD in each RG step depends on how accurately the environment is represented.
- ▶ $\rho^{(N)} \neq \rho_L \otimes \rho_R$
- ▶ For a pure Ψ_T : $s_L = s_R$
- ▶ Kullback-Leibler relative quantum entropy:

$$K(\rho_L || \sigma_L) \equiv \text{Tr}(\rho_L \ln \rho_L - \rho_L \ln \sigma_L),$$

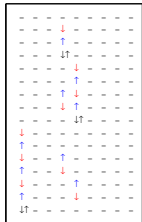
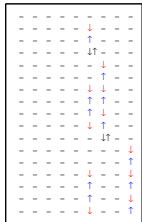
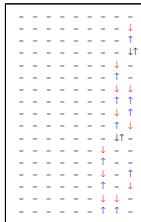
where ρ_L and σ_L denote reduced density matrices of the left block corresponding to two different right (environment) blocks.

- ▶ K measures how the system (left) block reduced density matrix changes as we change the environment.
- ▶ Optimize environment block based on Kullback-Leibler entropy.

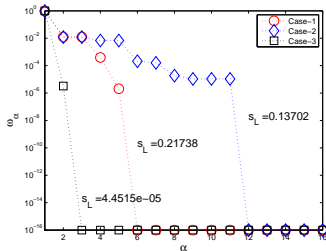
Example: LiF 6/12, orbitals 1,2,3 are the HF orbitals.



Consider three different basis sets: M_r

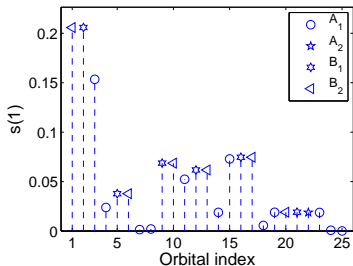


The reduced density matrix of the $L = l + 1$ subsystem depends on the basis states used for the $R = 1 + r$ environment:

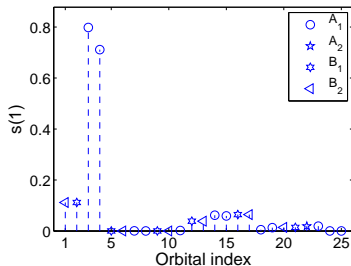


Efficient construction of the active space

The larger the entropy value for a given orbital the larger its contribution to the total correlation energy. Example LiF (6/25):



$r=3.05$



$r=13.7$

CAS-vector \equiv ordering sites with decreasing site entropy values.

Include orbitals with largest entropies in the expansion of the active space.

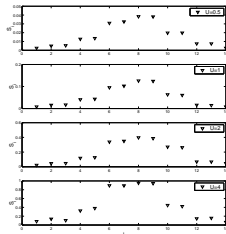
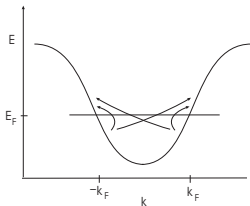
CI-based Dynamically Extended Active Space procedure

Change of basis and entanglement

$$\mathcal{H} = -t \sum_{j=1, \sigma}^N \left(c_{j, \sigma}^{\dagger} c_{j+1, \sigma} + c_{j+1, \sigma}^{\dagger} c_{j, \sigma} \right) + U \sum_{j=1}^N n_{j, \uparrow} n_{j, \downarrow}$$

$$\mathcal{H} = \sum_{k \sigma} \epsilon(k) c_{k \sigma}^{\dagger} c_{k \sigma} + \frac{U}{N} \sum_{k_1, k_2, k_3} c_{k_1 \uparrow}^{\dagger} c_{k_2 \downarrow}^{\dagger} c_{k_3 \downarrow} c_{k_1 + k_2 - k_3 \uparrow}$$

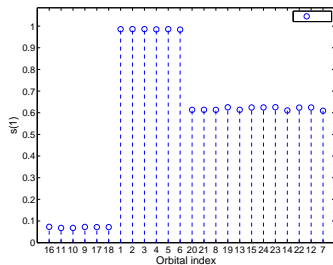
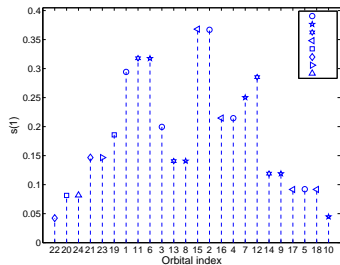
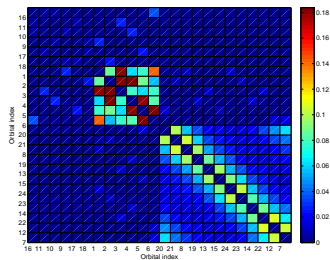
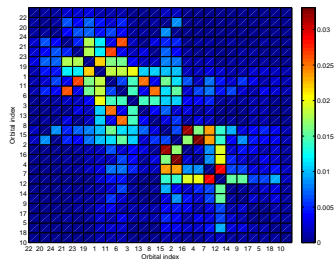
$\epsilon(k) = \sum_r e^{-ikr} t(r)$, where $k_i = (2\pi n)/N$, $-N/2 < n \leq N/2$.
 $T_{ij} = -2t \cos(k_i) \delta(i - j)$ and $V_{ijkl} = (U/N) \delta(i + j - k - l)$



real space: $U = 0, s_i = \ln 4$; $U \rightarrow \infty, s_i = \ln 2$.

k -space: $U = 0, s_i = 0$; $U \rightarrow \infty, s_i = \ln 4$. Ö.L., J. Sólyom, PRB (2003)

Entanglement pattern for a Be ring at $r = 2.15$ with canonical and localized basis



Basis states transformation applied to the Hamiltonian

There are two ways to implement the basis transformation: one based on the state and the other based on the Hamiltonian.

$$H = \sum_{ij} T_{ij} c_i^\dagger c_j + \sum_{ijkl} V_{ijkl} c_i^\dagger c_j^\dagger c_k c_l,$$

The function $E(U)$ can be expressed as

$$E(U) = \sum_{ij} \tilde{T}(U)_{ij} \langle c_i^\dagger c_j \rangle + \sum_{ijkl} \tilde{V}(U)_{ijkl} \langle c_i^\dagger c_j^\dagger c_k c_l \rangle \text{ with}$$

$$\tilde{T}(U) = UTU^\dagger$$

$$\tilde{V}(U) = (U \otimes U) V (U \otimes U)^\dagger.$$

The correlation functions $\langle c_i^\dagger c_j \rangle$ and $\langle c_i^\dagger c_j^\dagger c_k c_l \rangle$ are calculated with respect to the original state and are not dependent on the parameters in U . With the function $E(U)$ in this form, its gradient can be calculated explicitly. Both quantities can be evaluated efficiently for different parameter sets U .

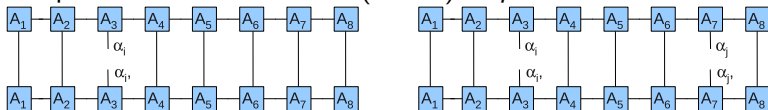
One- (ρ_i) and two-orbital ($\rho_{i,j}$) reduced density matrix

$$|\psi\rangle = \sum_{\alpha_1, \dots, \alpha_N} C_{\alpha_1, \dots, \alpha_N} |\alpha_1 \dots \alpha_N\rangle,$$

- $\rho_{i,j}$ is calculated by taking the trace of $|\Psi\rangle\langle\Psi|$ over all local bases except for α_i and α_j , the bases of sites i and j , i.e.,

$$\rho_{i,j}([\alpha_i, \alpha_j], [\alpha'_i, \alpha'_j]) = \sum_{\substack{\alpha_1, \dots, \cancel{\alpha_i}, \dots, \\ \alpha_j, \dots, \alpha_N}} C_{\alpha_1, \dots, \alpha_i, \dots, \alpha_j, \dots, \alpha_N} C_{\alpha_1, \dots, \alpha'_i, \dots, \alpha'_j, \dots, \alpha_N}^*$$

- In the MPS representation, calculation of ρ_{ij} corresponds to the contraction of the network except at sites i and j . The computational cost scales as $(N-2)m^3q^3$



- This can be decomposed as a sum of projector operators based on the free variables α_i and α_j .
- ρ_i and $\rho_{i,j}$ can be constructed from operators describing transitions between single-site basis states.

2-site density matrix and generalized correlation functions

Transitions between states of a q -dimensional local Hilbert space:

$$\mathcal{T}_i^{(m)} = \bigotimes_{j=1}^{i-1} \mathbb{I} \otimes \mathcal{T}^{(m)} \otimes \bigotimes_{j=i+1}^L \mathbb{I}.$$

where $(\mathcal{T}^{(m)})_{k,l} = \delta_{(l+q[k-1]),m}$ for $m = 1 \dots q^2$.

Example spin-1/2 boson (qbit):

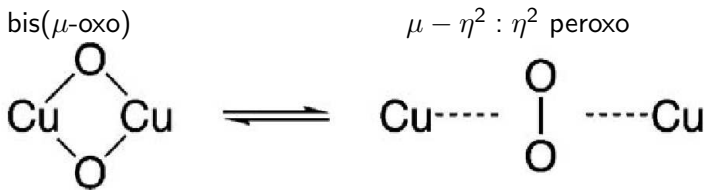
	\downarrow	\uparrow
\downarrow	$\mathcal{T}_i^{(1)}$	$\mathcal{T}_i^{(2)}$
\uparrow	$\mathcal{T}_i^{(3)}$	$\mathcal{T}_i^{(4)}$

$\mathcal{T}_i^{(1)}$	$-S_i^z + \frac{1}{2}\mathbb{I}$
$\mathcal{T}_i^{(2)}$	S_i^-
$\mathcal{T}_i^{(3)}$	S_i^+
$\mathcal{T}_i^{(4)}$	$S_i^z + \frac{1}{2}\mathbb{I}$

ρ_{ij}	$\downarrow\downarrow$	$\downarrow\uparrow$	$\uparrow\downarrow$	$\uparrow\uparrow$
$\downarrow\downarrow$	$\mathcal{T}^{(1)}\mathcal{T}^{(1)}$			
$\downarrow\uparrow$		$\mathcal{T}^{(1)}\mathcal{T}^{(4)}$	$\mathcal{T}^{(2)}\mathcal{T}^{(3)}$	
$\uparrow\downarrow$		$\mathcal{T}^{(3)}\mathcal{T}^{(2)}$	$\mathcal{T}^{(4)}\mathcal{T}^{(1)}$	
$\uparrow\uparrow$				$\mathcal{T}^{(4)}\mathcal{T}^{(4)}$

Quantum chemistry (some 40 electrons on 40 orbitals)

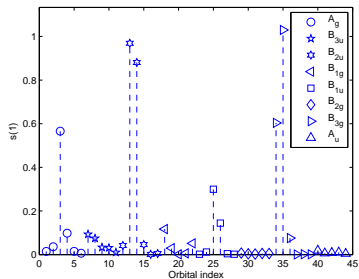
Example: Task to determine the electronic structure of the binuclear oxo-bridged copper clusters



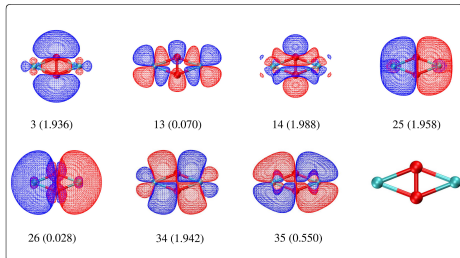
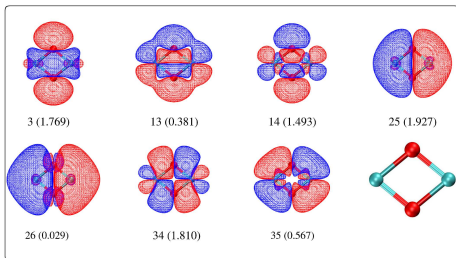
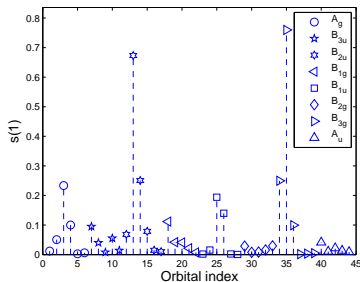
- ▶ CASSCF calculations yield a qualitative wrong interpretation of the energy difference between different isomers.
- ▶ Too large active space required to get qualitatively correct picture for standard QC methods.
- ▶ open d shell problem
- ▶ K.H. Marti, I.Malkin Ondik, G. Moritz, and M. Reiher, *J. Chem. Phys.* **128**, 014104 (2008).
Y. Kurashige, and T. Yanai, *J. Chem. Phys.* **130**, 234114 (2009).
T. Yanai, Y. Kurashige, E. Neuscamman, and G.K.-L. Chan, *J.Chem.Phys.* **132**, 024105 (2010).
G. Barcza, Ö. Legeza, K. H. Marti, and M. Reiher, *Phys. Rev. A.* **83**, 012508 (2011).

Site entropy profile \rightarrow highly entangled orbitals

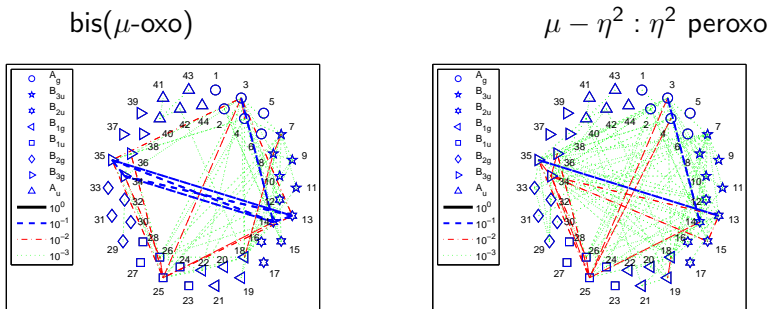
bis(μ -oxo)



$\mu - \eta^2 : \eta^2$ peroxo



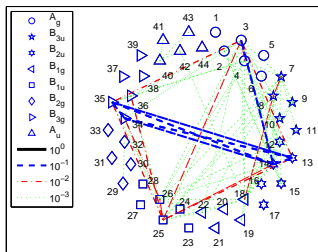
Entanglement picture of the two isomers



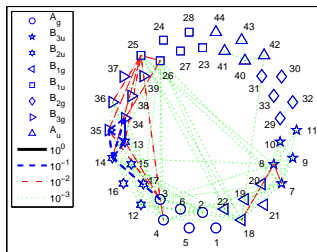
- ▶ peroxo: orbital pairs 3–14 and 13–35 are highly entangled
→ bonding and anti-bonding orbitals → the O–O bond is intact
- ▶ bis(μ -oxo): all five orbitals 3, 13, 14, 34, and 35 are entangled
→ four equivalent Cu–O bonds
- ▶ O–O bond breaking process → transition from the peroxo to the bisoxo isomer
- ▶ **Mutual information + DMRG → relative energy of the two-isomers**

Entanglement localization, example for bis(μ -oxo)

energetical ordering

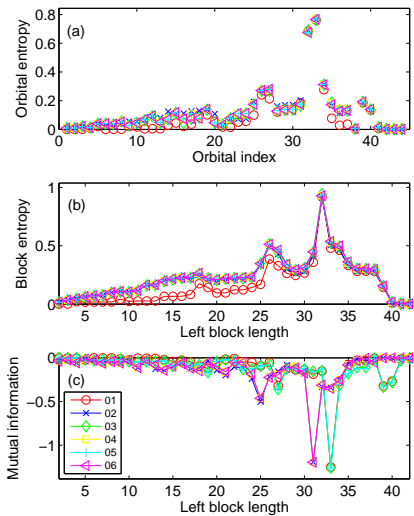
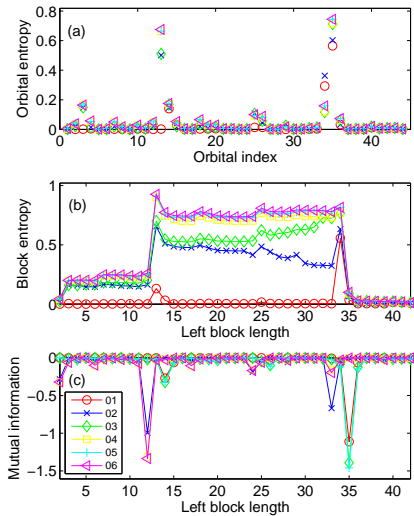


optimized ordering



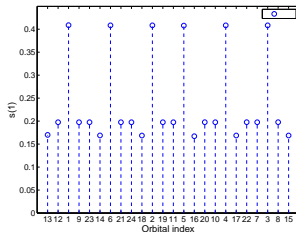
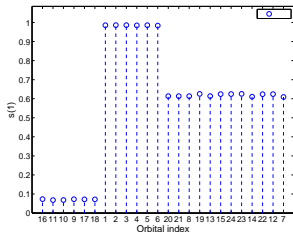
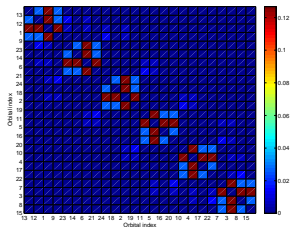
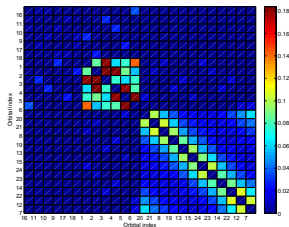
- ▶ Reordering orbitals by minimizing the entanglement distance:
$$\hat{l}_{\text{dist}} = \sum_{i,j} l_{i,j} \times |i - j|^\eta,$$
- ▶ Apply spectral graph theory: the vector $x = (x_1, \dots, x_N)$ is the solution that minimizes $F(x) = x^\dagger Lx = \sum_{ij} l_{i,j} (x_i - x_j)^2$, with $\sum_i x_i = 0$ and $\sum_i x_i^2 = 1$, and the graph Laplacian is $L = D - I$ with $D_{i,i} = \sum_j l_{i,j}$.
The second eigenvector of the Laplacian is the Fiedler vector.
Sorting elements of the Fiedler vector \rightarrow optimal ordering.

Entanglement localization



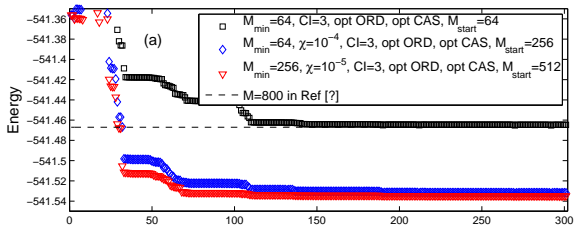
- ▶ Height and width of $S(l)$ can be reduced significantly.
- ▶ Computational cost is proportional to $\sum_l S(l)$.

Sorting elements of the Fiedler vector \rightarrow optimal ordering.



Mutual information and site entropy for the ground state of a **ring cluster** built from six Be atoms at the equilibrium bond length $d = 2.15$ and at a stretched geometry $d = 3.30$.

Relative energy of the isomers: a notebook calculation



Fixed number of block states vs DBSS
Dynamic Block State Selection

$$s_L(l+1) - s_L^{\text{Trunc}}(l+1) < \chi$$

- ▶ DBSS guarantees that the number of block states are adjusted according to the entanglement between the DMRG blocks and the a priori defined accuracy can be reached.
- ▶ Dynamically Extended Active Space (CI-DEAS)

method	ΔE
Reference energies	
CASSCF(16,14)	1
CASPT2(16,14)	6
bs-B3LYP	221
RASPT2(24,28)	120
Previously published DMRG energies	
[1],DMRG(26,44)[$m=800$]	78
[2],DMRG(32,62)[$m=2400$]	149
[3],DMRG(28,32)[$m=2048$]-SCF	107
[3],DMRG(28,32)[$m=2048$]SCF/CT	113
DMRG energies from this work	
DMRG(26,44)[$64/256/10^{-4}$]	111
DMRG(26,44)[$256/512/10^{-4}$]	115
DMRG(26,44)[$256/1024/10^{-4}$]	113
DMRG(26,44)[$256/512/10^{-5}$]	113
DMRG(26,44)[$256/1024/10^{-5}$]	113

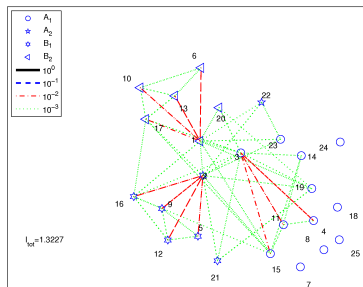
M. Reiher *et al*, *J. Chem. Phys.* **128**, (2008).
T. Yanai *et al*, *J. Chem. Phys.* **130**, (2009).
G.K.-L. Chan *et al*, *J.Chem.Phys.* **132**, (2010).

Part IV

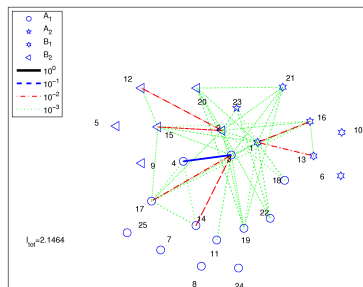
Higher dimensional networks

- ▶ Tree Tensor Network State (TTNS) algorithm
 - Multiply connected networks
 - Structure of the network
 - Optimization of the network topology
 - TTNS study of the avoided crossing in LiF

Entanglement \rightarrow Multiply connected networks



LiF at $r=3.05$



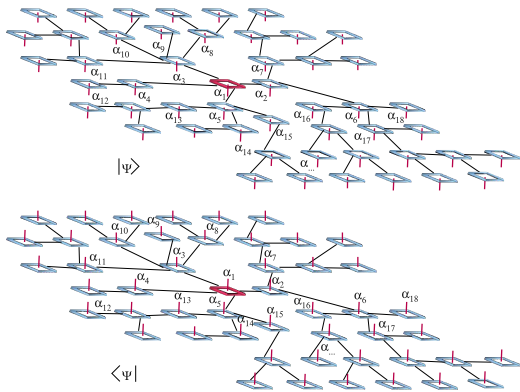
LiF at $r=13.7$

Rissler, White, Noack, ECP (2006)
Murg, Verstraete, Schneider, Nagy, Ö.L. (2013)

- ▶ DMRG \rightarrow Matrix product states, i.e. optimization along one-spatial dimension
- ▶ Need for an algorithm that reflects the entanglement topology of the problem \rightarrow Tensor Network State (TNS) methods
- ▶ Use tensors $A^i[\alpha]_{m_1 \dots m_z}$ where z is the coordination number

The two-dimensional network

A tree tensor network in which all sites in the tree represent physical orbitals (red lines) and in which entanglement is transferred via the virtual bonds that connect the sites (black lines).



Example: each node is represented by a tensor of order z_i and the vertical line denotes the physical index α_i . The central node is

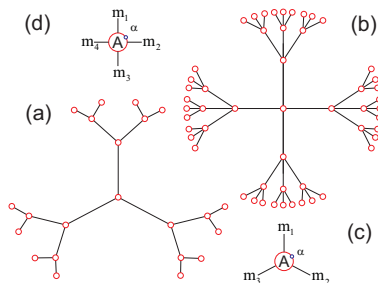
Tree Tensor Network State (TTNS)

$$|\Psi\rangle = \sum_{\alpha_1, \dots, \alpha_N} C_{\alpha_1 \dots \alpha_N} |\alpha_1, \dots, \alpha_N\rangle.$$

$C_{\alpha_1 \dots \alpha_N}$ describe a tree tensor network, i.e., they emerge from contractions of a set of tensors $\{A^1, \dots, A^N\}$, where

$$A^i [\alpha]_{m_1 \dots m_z},$$

is a tensor at each vertex i of the network, with z virtual indices $m_1 \dots m_z$ of dimension D and one physical index α of dimension q , with z being the coordination number of that site.



Vidal, Corboz (2009);

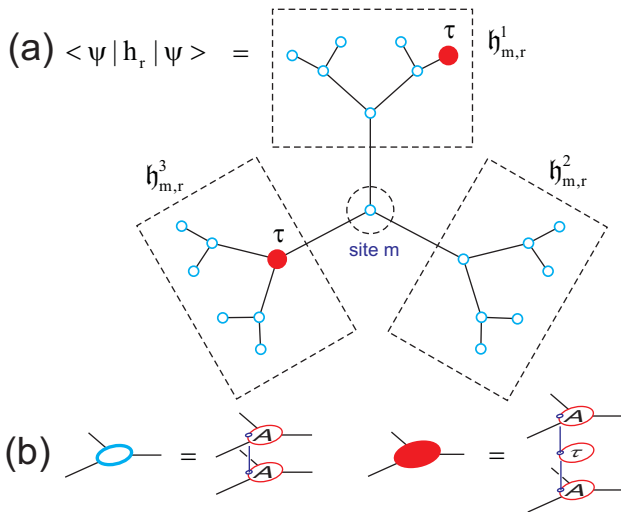
Murg, Verstraete, Ö.L., Noack (2010);

Nakatani, Chan (2013)

Structure of the network

- The coefficients $C_{\alpha_1 \dots \alpha_N}$ are obtained by contracting the virtual indices of the tensors.
- The structure of the network can be arbitrary.
- The coordination number can vary from site to site.
- The only condition is that the network is bipartite, i.e., by cutting one bond, the network separates into two disjoint parts.
- For $z = 2$, the one-dimensional MPS-ansatz used in DMRG is recovered.
- Entanglement is transferred via the virtual bonds that connect the sites.
- For $z > 2$ the number of virtual bonds required to connect two arbitrary sites scales logarithmically with the number of sites N , whereas the scaling is linear in N for $z = 2$.
- The maximal distance between two sites, 2Δ , scales logarithmically with N for $z > 2$.

Tree Tensor Network State (TTNS)



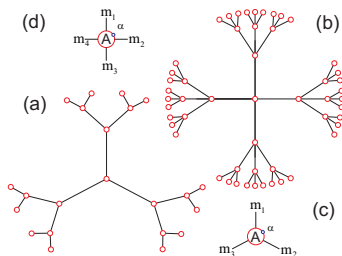
Tensor topology optimization: $\sum_{ij} l_{ij} \times d_{ij}^n$

l_{ij} is model dependent:

- ▶ depends on T_{ij} and V_{ijkl} interaction strengths
- ▶ depends on the choice of basis
- ▶ major aim: could we optimize basis on-the-fly (different approaches are under investigations, Chan, Murg, Verstraete, Ö.L., Krümmov, Eisler, Schneider); unsolved problem

d_{ij} depends on the tensor topology

- ▶ a possible solution: TTNS with site dependent coordination number z_i .



Number of sites in the tree:

$$N = 1 + z \sum_{j=1}^{\Delta} (z-1)^{j-1} = \frac{z(z-1)^{\Delta} - 2}{z-2}$$

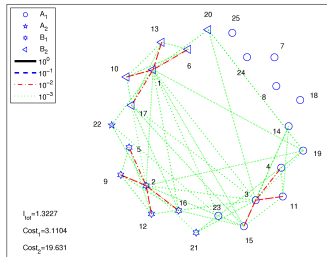
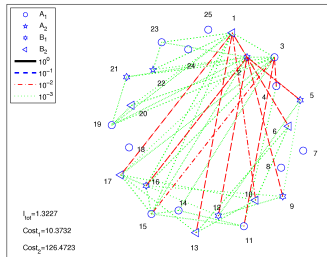
The maximal distance between two orbitals, 2Δ , scales logarithmically with N for $z > 2$.

Tensor topology optimization: $\sum_{ij} l_{ij} \times d_{ij}^n$ (Ex. LiF 6/25)

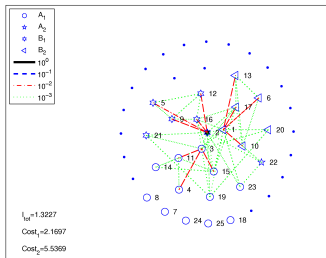
Energetical ordering (MPS)

$$d_{ij} = |i - j|$$

Entanglement localization (MPS)



Tree Tensor Network State (TTNS)

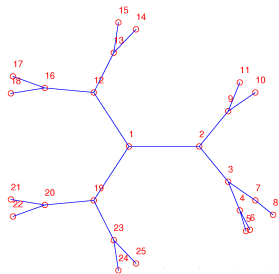


Optimization of the sweeping

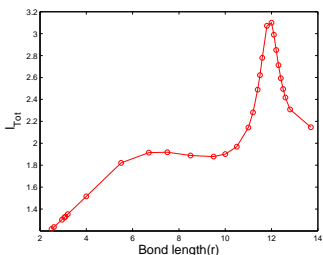
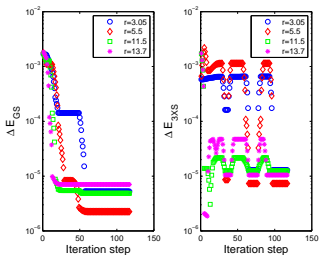
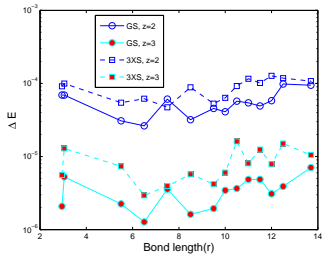
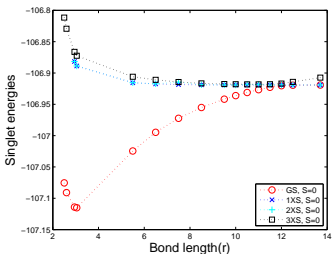
In case of the tree-network, there is more freedom to choose the optimal sweeping procedure, i.e., to choose the optimal path through which the network is traversed.

We sweep through the network by going recursively back and forth through each branch. Therefore, according to the labeling of the orbitals on the lattice shown in the figure one sweep goes through the orbitals:

1 2 3 4 5 4 6 4 3 7 8 7 3 2 9 10 9 11 9 2 1 12 13 14 13 15 13 12
16 17 16 18 16 12 1 19 20 21 20 22 20 19 23 24 23 25 23 19.



TTNS study of the avoided crossing in LiF (6/25)



V. Murg, F. Verstraete, R. Schneider, P. Nagy, Ö. L. (2014)