Tensor methods and entanglement measurements for models with long-range interactions

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- Thorsten Röhwedder and Reinhold Schneider (Tu-Berlin)
- Christian Krumnow, Jens Eisert, Edoardo Fertitta, Beate Paulus (Fu-Berlin)

Computational Challenges in Nuclear and Many-Body Physics, Nordita, Stockholm, 19.09.2014

- R. Feynman (1985): simulating quantum systems on classical computers takes an amount of time that scales exponentially with size of system, while quantum simulations can scale in polynomial time with system size.
- ► Tensor network states as low-rank approximations of high-dimensional tensor spaces → can provide efficient simulations on classical computers
- Major aim: no need to build expensive laboratories and experimental environments to design new materials and system just simulate them on computers
- In certain cases we can already reproduce and simulate experimental results

Properties of subsystems give information about the whole system

- Entanglement describes the quantum correlation between subsystems
- Mutual information: correlation between two selected subsystems embedded in a larger system

1. Multiply connected 2-dimensional entanglement network which describes physical properties of the system

 $\ensuremath{2}.$ Development of better numerical methods that reflect the entanglement pattern of the problem

Applications motivated by recent experiments

Cold atoms

► Fermionic alkaline earth atoms (AEA) in optical lattice potentials → quantum simulators of strongly correlated materials Gorshkov et al, Nat. Phys. 6, 289(2010)

In some cold atom systems the simplest realizations of strong correlation physics may have no solid state analog, for example SU(n), n > 2 Hubbard model
 → d and f band electrons Hermele *et al*, PRL 103, 135301 (2009)

 Exotic magnetic phases, i.e., chiral spin liquid Taie et al PRL 105, 190401 (2010).
 Quantum chemistry:

► Open d-shell properties → quantum chemistry of transition metal oxides Reiher, Chimia 63, 140 (2009)

Interacting 1D system

$$\mathcal{H} = t \sum_{i,\sigma} \left[c_{i+1,\sigma}^{\dagger} c_{i,\sigma} + h.c \right] + \frac{U}{2} \sum_{\sigma \neq \sigma'} \sum_{i} n_{i,\sigma} n_{i,\sigma'}.$$

on-site interaction U, nearest-neighbour hopping $t, \sigma = 1, \ldots, n$,

fermionic anticommutation relations

SU(4) lattice 1/3-filling

- SU(n) Hubbard model
 with integer No. of e⁻ on each site
 d and f band electron systems: to take into account the band
 (orbital) degeneracy
- Multiband systems



Heisenberg model

Honerkamp, Hofstetter PRL 92 170403



Brief historical overview (incomplete list)

- Renormalization Group (Kadanoff transformation) (1966)
- Block Renormalization Group (BRG) method Pfeuty(1978)
- Numerical Renormalization Group (NRG): Wilson(1975)
- Density Matrix Renormalization Group (DMRG): White(1992)
 - Dynamical DMRG (DDMRG): Jeckelmann(2002), Hallberg(1995),...
 - 2D-DMRG:

Noack, White, and Scalapino (1994,1996), Xiang(2000(2000)), McCulloch(2001)...

- Transfer Matrix DMRG: Batista (1998), Hallberg (1999), Nishino(1995), Moukouri(1996), Peschel(1998),...
- Momentum space version of DMRG (k-DMRG): Xiang(1996), Nishimoto, Noack(2002), Legeza, Sólyom(2003),...
- Quantum chemistry version of DMRG (QC-DMRG): White(1999), Mitrushenkov(2001), Chan(2002), Legeza(2002), Reiher(2005), Zgid(2006), Yanai(2008), Xiang(2010),...
- Time-dependent DMRG (t-DMRG): Schmitteckert(2004), Cirac, Verstraete(2004), Vidal, Schollwoeck (2004), Daley, White (2004), Manmana, Noack(2005), ...

Brief historical overview

Matrix Product State (MPS):

Östlund, Rommer(1995), Cirac, Verstraete(2004), Vidal (2003), Oseledets(2009), ...

Tensor Network Sates(TNS):

Cirac, Verstraete(2004), Vidal (2003), Orus(2005), Eisert(2005), Hackbush(2010),...

- Projected Entangled-Pair State (PEPS): Cirac, Verstraete(2004)
- Infinite Projected Entangled-Pair State (iPEPS): Jordan, Orus, Vidal, Verstraete, Cirac(2009) Corboz, White, Vidal, Troyer (2011), ...
- Multiscale entanglement renormalization algorithm (MERA):

Vidal (2007), Coborz (2009)

2D-MERA:

Evenbly, Vidal (2009)

▶ ...

Some useful reviews, also see additional references therein

- Density Matrix Renormalization: A New Numerical Method in Physics, Eds. I. Peschel, X. Wang, M. Kaulke, and K. Hallberg, ,Springer, 1999.
- 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.
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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.; ODEN, J.; Souganidis, P.; Tveito, A. (Eds.) Springer 2013 ISBN 978-3-540-70530-7
- O. Legeza, T. Röhwedder, R. Schneider, Sz. Szalay, arxiv:1310.2736 (2013).
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- ▶ J. Eisert, M. Cramer, M.B. Plenio, Rev. Mod. Phys. 82, 277 (2010).
- http://tagung-theoretische-chemie.uni-graz.at/en/past-workshops/workshop-2014/
- http://ldqs.iyte.edu.tr/program/

Topics to be covered

- 1. Motivation and former approaches: Model Hamiltonian, i.e., problem to solve Problem in the language of tensor factorization
- 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 \rightarrow Entanglement
 - Optimizing the algorithms Legeza, 2003; Rissler, 2006
 - Efficient construction of active spaces Legeza,2003
 - Description of bond formation and breaking procedures Boguslawski,2012
- 4. Four-Component DMRG (4c-DMRG) Knecht, Reiher, Legeza, 2013
- 5. MPS based on-the-fly basis optimization Krumnow, Schneider, Legeza, Eisert, 2014
- 6. MPS and TNS on kilo-processor architectures: smart hybrid CPU-GPU implementation Nemes, Barcza, Nagy, Legeza, Szolgay, 2014

Nonlocal Interactions, Quantum Chemistry and Momentum space

Higher dimensional system can be mapped to a 1-d chain local interactions \rightarrow non-local interactions



General nonlocal fermionic Hamiltonian

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

Describes:

- quantum chemistry (post-Hartree-Fock)
- momentum-space Hamiltonians
- fractional quantum Hall
- Iong-range Hamiltonians in real space, ...

General case: Quantum Chemistry application (QC-DMRG)

Idea: 1-d chain is built up from the molecular orbitals that were obtained, e.g., in a suitable mean-field or MCSCF calculation (MOLPRO program package). Ex.: H₂O in double-ζ(DZ) basis. White and Martin (1999), Chan (2002) O.L. (2002), Reiher(2005), ...



- Carry out "normal" DMRG (with nonlocal, long-range interactions)
- CI method: Slater determinants by removing one (S), two (D), three (T) or four (Q) electrons form the HF orb.:

$$\Psi_{CI} = a_0 \Phi_{SCF} + \sum_S a_S \Phi_S + \sum_D a_d \Phi_D + \sum_T a_t \Phi_T + \dots$$

► MPS wavefunction can provide CI coefficients Reiher (2011).

Hamiltonian of the interacting electron system

The system is described by the Hamiltonian, for example,

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

- *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 H.

The problem in the language of tensor factorization

▶ For a system with *N* molecular orbitals: ●●●...●

•
$$\Lambda^{(1,2,\ldots,N)} = \bigotimes_{i=1}^{N} \Lambda^{(i)}$$
 with $\dim \Lambda^{(1,2,\ldots,N)} = \prod_{i=1}^{N} \dim \Lambda^{(i)} = q^{N}$

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

► U^(1,2,...,N)_{α1,α2,...αN,k} is a tensor of order N corresponding to the kth eigenstate of the N-orbital Hamiltonian



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

Example: N = 8

Tensor product approximations:

Matrix Product State (MPS) representation:

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

$$|\Psi\rangle \qquad \boxed{A^1 \qquad A^2 \qquad A^3 \qquad A^4 \qquad A^5 \qquad A^6 \qquad A^7 \qquad A^8}_{\alpha_1 \qquad \alpha_2 \qquad \alpha_3 \qquad \alpha_4 \qquad \alpha_5 \qquad \alpha_6 \qquad \alpha_7 \qquad \alpha_8}_{\varphi\Psi} \qquad \boxed{A^1 \qquad A^2 \qquad A^3 \qquad A^4 \qquad A^5 \qquad A^6 \qquad A^7 \qquad \alpha_8}_{A_i[m,m]_{q_i}}$$

 We can call this a network. Matrix product state (MPS) / Tensor Train (TT): Ostlund, Rommer (1995), Verstraete, Cirac (2004), Oseledets (2009), Hackbusch (2009) The problem in the language of tensor factorization

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

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





Transfer tensor:

Series of transfer tensors:

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

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

DMRG provides MPS wavefunction:

Density matrix renormalization group wavefunction: (White, 1992)



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.

Density Matrix Renormalization Group (DMRG) method [White, 1992]



1. Form and diagonalize the superblock Hamilton operator

$$|\Psi_{\mathrm{TG}}
angle = \sum_{lpha_l lpha_{l+1} lpha_{l+2} lpha_r} \psi_{lpha_l lpha_{l+1} lpha_{l+2} lpha_r} |\phi_{lpha_l}^{(l)}
angle \otimes |\phi_{lpha_{l+1}}^{(s_l)}
angle \otimes |\phi_{lpha_{l+2}}^{(s_r)}
angle \otimes |\phi_{lpha_r}^{(r)}
angle$$

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

- 2. Form a bi-partite representation $|\Psi_{\rm TG}\rangle = \sum_{ij} \psi_{i,j} |\phi_i^{(L)}\rangle |\phi_j^{(R)}\rangle$
- 3. Form reduced subsystem density matrix $\rho_{i,i'}^{(L)} = \sum_{j} \psi_{i,j} \psi_{i',j}^*$
- 4. Diagonalize $\rho \to \omega_{\alpha}$ 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: $c_i \Rightarrow Oc_i O^{\dagger}$

DMRG infinite- and finite-lattice algorithm



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

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

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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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, $\delta \varepsilon_{\rm sweep}$, is minimized by a successive application of the sweepings
- Truncation error: $\delta \varepsilon_{\rm TR} = 1 \sum_{\alpha=1}^{M} \omega_{\alpha}$
- ▶ For $\delta \varepsilon_{\text{sweep}} \rightarrow 0$, $\delta E_{\text{rel}} = Const \times \delta \varepsilon_{\text{TR}}$ (Ö.L and G. Fáth, PRB 1996).
- DMRG is a variational method
- DMRG is a data-sparse representation of the wavefunction

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

- 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 $\operatorname{Tr} \rho_{\gamma} = 1$.

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

Dynamic Block State Selection (DBSS) procedure

Optimal truncation scheme: $\delta \varepsilon_{TR} < \epsilon$ fixed in advance $\rightarrow M$ is chosen accordingly in every step Example from 2002: DBSS approach applied on F₂ (D_{2h}) (18/18) $\Lambda_{FCI} = (2N)!/[(2N - N_e)!N_e!] = 9075135300$ $\Lambda_{DMRG} = M_l \times 4 \times 4 \times M_r = 28800000 (M_l = 1200, Mr = 1500)$ sparsity $\simeq 315$ $\Lambda_{DMRG} = M_l \times 4 \times 4 \times M_r = 7680 (M_l = 120, Mr = 4)$ sparsity $\simeq 1181658$ Ö.L., Roder, Hess, Phys Rev B (2002)



Dynamic Block State Selection (DBSS) procedure

Example 1d-Hubbard model:

$$\mathcal{H} = \sum_{i\sigma} t(c^{\dagger}_{i\sigma}c_{i+1\sigma} + c^{\dagger}_{i+1\sigma}c_{i\sigma}) + U\sum_{i} c^{\dagger}_{i\uparrow}c_{i\uparrow}c^{\dagger}_{i\downarrow}c_{i\downarrow} \,.$$

 $\Lambda_{SB} = \Lambda^{(L)} \otimes \Lambda^{(R)},$



Block entropy, *S*, and $\ln(\dim \Lambda)$, $\ln(\dim \Lambda_{SB})$ as a function of iteration steps for the half-filled 1-d Hubbard model with N = 80 for U = 1 with fixed number of block states (M = 512) using PBC.



Parameter β as a function of rescaled iteration step using DBSS approach for $TRE_{max} = 10^{-4}$, $M_{min} = 16$, U = 1, N = 40, 60, 80.

 $\beta \equiv \ln(\dim \Lambda) - S.$

Dynamic Block State Selection (DBSS) procedure

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

$$ho^{(L)} = oldsymbol{p}_{ ext{kept}}
ho^{(L)}_{ ext{kept}} + (1 - oldsymbol{p}_{ ext{lost}})
ho^{(L)}_{ ext{lost}} \,,$$

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

$$\chi \leq S(
ho) - p_{ ext{kept}} S(
ho_{ ext{kept}}) - (1 - p_{ ext{kept}}) S(
ho_{ ext{lost}}) \,,$$

- \blacktriangleright In DMRG the atypical subspace is neglected \rightarrow loss of information.
- truncation scheme: χ ≡ S(ρ) − S(ρ_{kept}) < ε fixed in advance → M is chosen accordingly in every step.</p>
 - Ö. L. and Sólyom, PRB(2004)

Entropy reduction by forming an enlarged system:

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

Obtained correlation in one RG step:

 $I_{L}(l) = s_{L}(l+1) - s_{L}(l) - s_{l+1} \qquad 1 \le l < N-1$

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





▶ For $L = N - 2 \rightarrow r = M_L = M_R = 1$, correlation functions can be calculated very quickly

A priory 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



Ö.L., Sólyom, PRB (2003)

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: $\rho_{i,i'}^{(L,R)} = \sum_j \psi_{ij} \psi_{ij}^* \psi_{i'j}^*$
- 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 ⇒entangled state: non-local property of quantum mechanics. Example: $1/\sqrt{2}(|\downarrow\rangle|\uparrow\rangle - |\uparrow\rangle|\downarrow\rangle)$
- Neumann entropy: $s(\rho^{\gamma}) = -\operatorname{Tr}(\rho^{\gamma} \ln \rho^{\gamma}), \gamma \equiv L, R$
- $|\Psi_{T}
 angle$ pure state $ightarrow s(
 ho^{L}) = s(
 ho^{R})$
- ▶ In general, $\rho^{L} = Tr_{R}$ and $\rho^{R} = Tr_{L}$ are in mixed state
- If $\omega_i = 1/M$ maximally mixed state
- In general $\rho^{(N)} \neq \rho_L \otimes \rho_R$

Entanglement

- ► Rényi entropy:s(ρ_i)_α = 1/(1-α) ln Trρ_i^α full spectrum of ρ_α (Calabrese) related to scaling of algorithms based on matrix product states(Schuch)
- Neumann entropy: $s_{\alpha \to 1}(\rho_i) = -\text{Tr}(\rho_i \ln \rho_i), i \equiv L, R$
- Single copy entanglement: $S_{\infty}(\rho_i) \equiv \ln \max(\rho_i)$
- $|\Psi_{T}
 angle$ pure state ightarrow $s(
 ho_{L}) = s(
 ho_{R})$
- Kullback-Leibler-relative entropy:

$$K(\rho||\sigma) \equiv \operatorname{Tr}(\rho \ln \rho - \rho \ln \sigma),$$

where ρ and σ reduced density matrix for the left block corresponding to two different environment.

- For more then two subsystems: Mutual entropy: $s(\rho_{AB}) = s(\rho_A) + s(\rho_B) - I$ where I describes correlation between A and B.
- $I = 0 \rightarrow A$ and B are uncorrelated.

▶ 1D

- Noncritical Systems: correlation functions decay exponentially Entropy constant: S(l) ~ const.
- Critical Systems: entropy diverges logarithmically (Vidal et al., 2003)

 $S(I) \sim \log I$ fo a subsystem of length I conformally invariant system:

$$S(l) = (c/6) \ln \left[\frac{2L}{\pi a} \sin(\frac{\pi l}{L}) \right] + g + c'_1$$
 (openBCs)

 \rightarrow conformal charge

2D

Entropy area "law" (Srednicki, 1993)

 $S(l) \gtrsim L^{d-1}$ L^{d-1} : area of boundary

Critical systems:

 $S(I) \gtrsim L^{d-1} \ln I \longrightarrow \text{required } m :\sim e^{S(I)} \sim e^{L^{d-1}}$





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

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



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

Spatial structures: Block entropy

In Fourier space:

$$\tilde{s}(k) = \frac{1}{N} \sum_{l=0}^{N} e^{-ikl} s_N(l)$$

for discrete wave numbers, $k = 2\pi j/N$, $k \in (-\pi, \pi)$.



Peaks in $|\tilde{s}(k)|$ { Sólyom, Tincani, Noack (2007) position of soft modes in critical systems spatial inhomogeneity of the ground state

Mutual information: entanglement correlation



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



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

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



Entanglement picture of the two isomers



- ▶ peroxo: orbital pairs 3–14 and 13–35 are highly entangled \rightarrow bonding and anti-bonding orbitals \rightarrow 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
- \blacktriangleright O–O bond breaking process \rightarrow transition from the peroxo to the bisoxo isomer
- Mutual information + DMRG \rightarrow relative energy of the two-isomers

Entanglement localization, example for $bis(\mu$ -oxo)





• Reordering orbitals by minimizing the entanglement distance: $\hat{I}_{\text{dist}} = \sum_{i,j} I_{i,j} \times |i - j|^{\eta}$,

Apply spectral graph theory: Fiedler vector x = (x₁,...x_N) is the solution that minimizes F(x) = x[†]Lx = ∑_{ij} l_{i,j}(x_i - x_j)², with ∑_i x_i = 0 and ∑_i x_i² = 1, and the graph Laplacian is L = D − I with D_{i,i} = ∑_j l_{i,j}. The second eigenvector of the Laplacian is the Fiedler vector.

Entanglement localization







- 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) procedure

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**, (200 T. Yanai *et al*, J. Chem. Phys. **130**, (2009

G.K.-L. Chan et al, J.Chem.Phys. 132, (20

Chemical bond forming and breaking vs Entanglement



Boguslawski, Tecmer, Barcza, Legeza, Reiher, 2013

Part II

Higher dimensional networks

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

Entanglement \rightarrow Multiply connected networks



- \blacktriangleright DMRG \rightarrow Matrix product states, i.e. optimization along one-spatial dimension
- \blacktriangleright Need for an algorithm that reflects the entanglement topology of the problem \rightarrow Tensor Network State (TNS) methods
- Use tensors $A^{i}[\alpha]_{m_{1}...m_{z}}$ where z is the coordination number

The two-dimensional network

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

Tree Tensor Network State (TTNS)

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

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

$$A^{i}\left[\alpha\right]_{m_{1}\ldots m_{z}}$$

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



Vidal, Corboz (2009); Murg, Verstraete, Ö.L., Noack (2010,2014); Nakatani, Chan (2013) • The coefficients $C_{\alpha_1...\alpha_N}$ are obtained by contracting the virtual indices of the tensors.

- The structure of the network can be arbitrary.
- The coordination number can vary from orbital to orbital.

• 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 orbitals.

• For z > 2 the number of virtual bonds required to connect two arbitrary orbitals scales logarithmically with the number of orbitals N, whereas the scaling is linear in N for z = 2.

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

Tree Tensor Network State (TTNS)



Tensor topology optimization: $\sum_{ij} I_{ij} \times d_{ij}^{\eta}$

Iij 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., Krumnow, Eisert, Schneider); unsolved problem
- d_{ij} depends on the tensor topology
 - a possible solution: TTNS with orbital dependent coordination number z_i .



Number of orbitals in the tree:

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

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

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



Tree Tensor Network State (TTNS)



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)

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

$${m E}(U) = \sum_{ij} ilde{\mathcal T}(U)_{ij} \langle c_i^\dagger c_j
angle + \sum_{ijkl} ilde{\mathcal V}(U)_{ijkl} \langle c_i^\dagger c_j^\dagger c_k c_l
angle ext{ with }$$

$$\begin{split} \widetilde{\mathcal{T}}(U) &= U T U^{\dagger} \ \widetilde{\mathcal{V}}(U) &= (U \otimes U) \mathcal{V}(U \otimes U)^{\dagger}. \end{split}$$

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

Local mode transformation: black-box tool to improve basis (Krumnow,

Schneider, Legeza, Eisert, 2014

- Perform updates iteratively and adaptively, both in the MPS ansatz and in mode transformations. $A^{(1)} \xrightarrow{D^{(1)}} A^{(2)} \xrightarrow{D^{(2)}} A^{(3)} \xrightarrow{D^{(3)}} \cdots \xrightarrow{D^{(n-1)}} A^{(n)}$
- Consider a matrix-product state with physical dimension *d* and maximal bond dimension $D_{\max} = \max\{D^{(j)}\}$.
- For given $j \in \{1, \ldots, n-1\}$, minimize the energy by jointly optimizing the tensors $A^{(j)} \in \mathbb{C}^{D^{(j-1)} \times D^{(j)} \times d}$ and $A^{(j+1)} \in \mathbb{C}^{D^{(j)} \times D^{(j+1)} \times d}$ at sites j and j+1
- Jointly update $A^{(j)}$, $A^{(j+1)}$ with Hilbert space representation of mode transformations $U \in U(2 \log_2 d)$ on the respec physical legs of the tensors, optimizing the Schmidt-spe of $A_{opt}^{(j,j+1)}(U)$ over the cut j, j+1 and truncate. \blacksquare Update the operators with $U_{\mathsf{global}} := \mathbb{1} \oplus U \oplus \mathbb{1}$
- e.g. the Hamiltonian
 - $H \mapsto \tilde{H} := G(U_{\text{global}}) H G^{\dagger}(U_{\text{global}})$

exploiting their second quantized representation

$$\begin{array}{l} H(T, V) \mapsto \tilde{H} = H(\tilde{T}, \tilde{V}) \\ T \mapsto \tilde{T} := U_{\text{global}} T U_{\text{global}}^{\dagger} \\ V \mapsto \tilde{V} := (U_{\text{global}} \otimes U_{\text{global}}) V (U_{\text{global}}^{\dagger} \otimes U_{\text{global}}^{\dagger}) \end{array}$$

tions
$$G(U)$$

tive $e^{e^{e^{i - J}}}$ $A_{opt}^{(j,i+1)}$ $A_{opt}^{(j,i+1)}$
tive $e^{e^{e^{i - J}}}$ $A_{opt}^{(j,i+1)}$ $A_{opt}^{(j,i+1)}$

- Go to next site $j \mapsto j \pm 1$ and iterate.
- Build up a global non-trivial mode transformation by consecutive local mode transformations with overlapping support
- At some point, fix the basis (which has now been optimised to the MPS ansatz and not Renyi entropic qualifiers) and perform state-of-the art DMRG with large bond dimension.

Example from quantum chemistry: Be₆-ring

system

- Known to show strong correlation effects [7]
- 12 electrons in 24 spin-degenerate orbitals (d = 4)
- Calculation performed with low bond dimension: $D_{max} = 90$
- Use adaptive mode transformation minimizing $\|\Sigma_{j,j+1}(U_{\uparrow} \oplus U_{\downarrow})\|_1$ respecting spin conservation and one additional reordering based on the mutual information [7] at the end of the calculation

results

standard basis vs energy and entropies of converged states:

$$rac{E_{
m conv}-E_{
m GS}}{E_{
m GS}}=7 imes 10^{-3}$$

 $\sum_{j=1}^n S_1(
ho_{[j]})=20.65$

$$\sum_{i=1}^{n} rac{E_{
m conv}-E_{
m GS}}{E_{
m GS}} = 2 imes 10^{-1}$$

mutual information: $I(i,j) = S_1(\rho_{\{i\}}) + S_1(\rho_{\{j\}}) - S_1(\rho_{\{i,j\}})$





transformed basis

Four-Component Density Matrix Renormalization Group

- ▶ TIH with double group $C_{2\nu}$ symmetry (14 e / 94 spinors),
- DIRAC12(2012), a relativistic ab initio electronic structure program,
- including spin-orbit coupling,
- 4c-DMRG with max(M) \simeq 4500 5000, $\chi = 10^{-5}$



S. Knecht, M. Reiher, Ö Legeza (2013)

MPS and TNS on kilo-processor architectures:

Nemes, Barcza, Nagy, Legeza, Szolgay, 2014

- The most time-dominant step of the diagonalization can be expressed as a list of dense matrix operations
- A smart hybrid CPU-GPU implementation, which exploits the power of both CPU and GPU and tolerates problems exceeding the GPU memory size.
- A new CUDA kernel has been designed for asymmetric matrix-vector multiplication to accelerate the diagonalization
- Example: Hubbard model on Intel Xeon E5-2640 2.5GH CPU + NVidia K20 GPU:

1071 GFlops and ×3.5 speedup is reached. (Theoretical maximum is 1.17 TFlops)



Conclusion

- With DMRG(MPS) very large active spaces can be treated
- Number of orbitals in the tree-TNS:

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

and thus, the maximal distance between two orbitals, 2Δ , scales logarithmically with N for z > 2.

- ► Therefore, in the tree-TNS entanglement can be localized more efficiently than in the MPS 1d topology → lower tensor ranks but larger tensor orders (crossover in scaling)
- ► Local mode transformation: MPS based black-box tool to improve basis
- MPS and TNS algorithms can utilize the enormous computing capabilities of novel kilo-processor architectures (GPU and FPGA)