Adaptive mode transformations in fermionic tensor networks

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Non-local fermionic models are frequently encountered in physics, most prominently in quantum chemistry, but also when capturing quantum lattice systems. If strong correlations are present in the system, traditional numerical methods such as HF, CI or CC are very limited. In these cases tensor-network methods provide a way out at the cost of being more expensive. The long-range nature of the interaction of such systems, however, renders their straightforward numerical simulation using tensor-network methods difficult. When using a DMRG-based method, a suitable reordering of the orbitals will already reduce the computational effort. Still, one has more freedom to preprocess the Hamiltonian by means of suitable linear maps from one set of fermionic modes to another, aiming at minimising the entanglement present in the system. Here, we present an adaptive method that aims at combining advantages arising from suitable local mode transformations and matrix-product updates "on the fly" in an iterative fashion. Our **results** – both for lattice models and for systems in quantum chemistry – show that by including such local mode transformations and applying known reordering techniques, one finds good approximations of the ground state already for low bond dimensions and optimizes the entanglement structure present in the ground. In addition, we are able to recover global mode transformation from the local ones for medium sized systems.

Type of problem and setting

Consider interacting long-range Hamiltonians in second quantised form with finitely many fermionic modes

$$H = \sum_{i,j} T_{i,j} c_i^\dagger c_j + \sum_{i,j,k,l} V_{i,j,k,l} c_i^\dagger c_j^\dagger c_k c_l$$

with two-body interactions in terms of fermionic modes $(c_1, \ldots, c_n)$. Such systems can be strongly correlated and are encountered in

- **quantum chemistry** (open shell systems, bond formation and breaking, intermolecular forces, transition metal complexes),
- **lattice systems** (interacting lattice models such as Hubbard model).

Challenges

- Using the Jordan-Wigner transformation the problem can be mapped to a long-range spin model with Hilbert space $(\mathbb{C}^d)^{\otimes n}$ and treated with matrix-product approaches: But long range nature demands high matrix-product state-bond dimension.

Tensor network algorithms favour local Hamiltonians, but in general we have long range interactions

- How to exploit the entanglement structure?
- How to optimise the network?
- How to compute expectations efficiently?

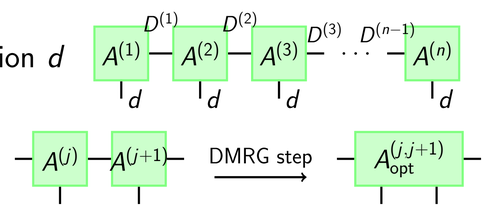
- Entanglement qualifiers depend strongly on the chosen ordering of sites and the choice of basis [1, 2, 3]. If **Renyi entropies** $S_\alpha(\rho_I)$, $\alpha \in (0,1)$, of subsystems $I \subset \{1, \ldots, n\}$ are small ("satisfy area laws" [4]), matrix-product states of low bond dimension can be found [5].
- "Preprocessing of Hamiltonian" seems desirable (see e.g. [6]), but how?

Idea

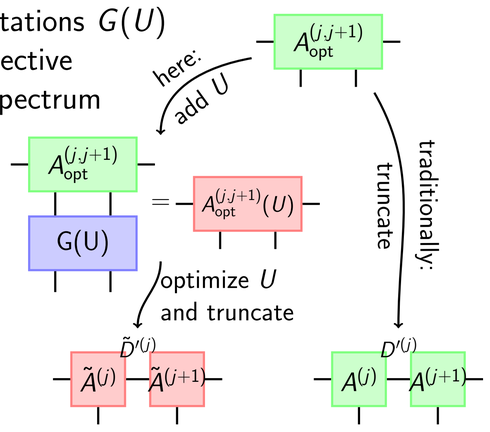
Combine the advantages of tensor network methods and suitable mode transformations

1. Unitary mode transformations can be performed easily on the level of the Hamiltonian and preserve the operator algebra: But they alter the Renyi entropy qualifiers and necessary bond dimensions largely.
2. Matrix-product state (MPS) updates capture correlations of the interacting model.

- Perform updates **iteratively and adaptively**, both in the MPS ansatz and in mode transformations.
- Consider a matrix-product state with physical dimension d and maximal bond dimension $D_{\text{max}} = \max\{D^{(j)}\}$.
- 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 representations $G(U)$ of mode transformations $U \in U(2\log_2 d)$ on the respective physical legs of the tensors, optimizing the Schmidt-spectrum of $A^{(j,j+1)}_{\text{opt}}(U)$ over the cut $j, j+1$ and truncate.
- Update the operators with $U_{\text{global}} := \mathbb{1} \oplus U \oplus \mathbb{1}$ e.g. the **Hamiltonian**
  $H \mapsto \tilde{H} := G(U_{\text{global}})\, H\, G^\dagger(U_{\text{global}})$
  exploiting their second quantized representation
  $H(T, V) \mapsto \tilde{H} = H(\tilde{T}, \tilde{V})$
  $T \mapsto \tilde{T} := U_{\text{global}}\, T\, U_{\text{global}}^\dagger$
  $V \mapsto \tilde{V} := (U_{\text{global}} \otimes U_{\text{global}})\, V\, (U_{\text{global}}^\dagger \otimes U_{\text{global}}^\dagger)$



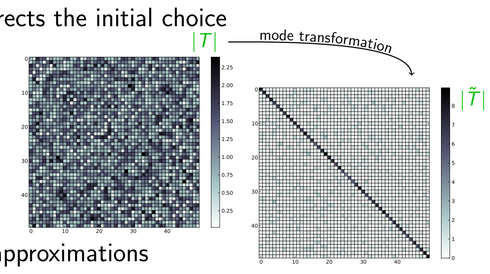
- Go to next site $j \mapsto j \pm 1$ and iterate.
- Build up a global non-trivial mode transformation by consecutive local mode transformations with overlapping support
- At some point, fix the basis (which has now been optimised to the MPS ansatz and not Renyi entropic qualifiers) and perform state-of-the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

Details on mode transformations

- The Hilbert space representation $G(U)$ decomposes into a direct sum over different particle number sectors $G(U) = \bigoplus_{i=0}^{2\log_2 d} G_i(U)$, where $G_i(U) \simeq \bigwedge^i U$ ($\bigwedge$ denotes the exterior product) and $\log_2 d$ amounts to the number of fermion-species in the system.
  E.g. d=2: $G_0(U) = 1$, $G_1(U) \simeq U$ and $G_2(U) = \det U = e^{i\phi}$, $\phi \in [0, 2\pi)$.
- If further symmetries are present U decomposes into different symmetry sectors $U = \bigoplus_\sigma U_\sigma$
  E.g. d=4 and spin conservation: $U = U_\uparrow \oplus U_\downarrow$ with $U_\sigma \in U(2)$.
- Optimization-goal: identify a basis in which maximal required bond dimension is minimal.
- Optimize $\|\Sigma_{j,j+1}(U)\|_\alpha$ or $S_\alpha(\rho_{[j]}(U))$ where $\Sigma_{j,j+1}(U)$ corresponds to Schmidt-spectrum of the U-transformed state when cut at j, $j+1$.
- Reduce optimization parameters by considering only relevant degrees of freedom for those target functions by optimizing over the right cosets $U(2\log_2 d) \backslash U(\log_2 d) \oplus U(\log_2 d)$.
  E.g. d=2: $\forall U \in U(2)/U(1) \oplus U(1) : U = e^{ix_1\sigma_z} e^{ix_2\sigma_y}$, optimize over x_1, x_2 brute-force.
  Or d=4: $U(4) \backslash U(2) \oplus U(2)$ has 8 free parameters. Use either gradient of $\|\Sigma_{j,j+1}(U)\|_4^4$ to improve convergence of optimization or exploit symmetry if present ($U(2)^2 \backslash U(1)^4$ needs 4 parameters).

Results

- Starting initially on purpose in a "wrong" basis, method auto-corrects the initial choice
  - case $V = 0$: mode transformations diagonalize T
  - case $V \neq 0$ and $D_{\text{max}} \approx 1$: recover HF orbitals
- If symmetries of the system are not hard-coded into the state, method identifies basis in which representing a state respecting this symmetry even for low D_{max} is possible.
- Improves basis of interacting systems for $D_{\text{max}} \gg 1$ beyond known techniques such that more accurate ground state approximations are possible.



Example from quantum chemistry: Be_6-ring

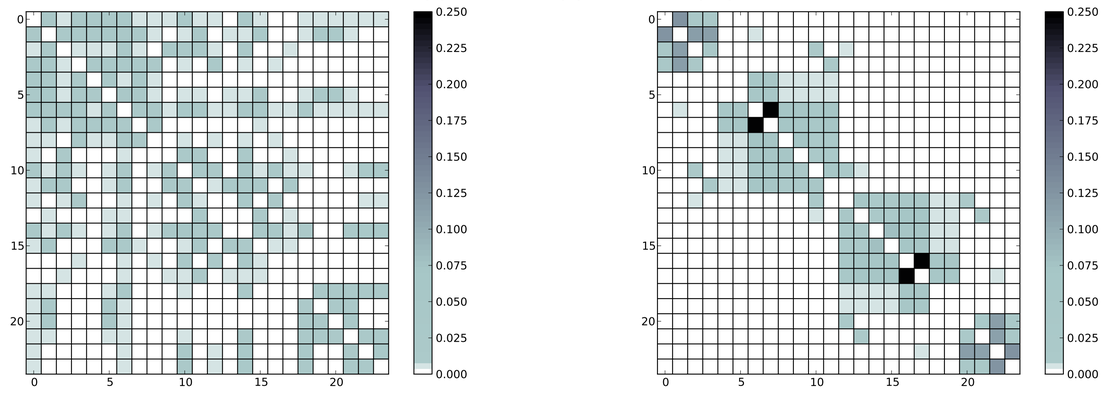
system

- Known to show strong correlation effects [7]
- 12 electrons in 24 spin-degenerate orbitals ($d = 4$)
- Calculation performed with low bond dimension: $D_{\text{max}} = 90$
- 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	transformed basis
energy and entropies of converged states:		
$\frac{E_{\text{conv}} - E_{\text{GS}}}{E_{\text{GS}}} = 7 \times 10^{-3}$		$\frac{E_{\text{conv}} - E_{\text{GS}}}{E_{\text{GS}}} = 2 \times 10^{-4}$
$\sum_{j=1}^{n} S_1(\rho_{[j]}) = 20.65$		$\sum_{j=1}^{n} S_1(\rho_{[j]}) = 10.88$

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



Conclusion and outlook

- Local mode transformation provide black-box tool to improve basis used in tensor-network calculations.
- Method not restricted to MPS, can be used to optimize trees or 2d-systems combined with fermionic networks [8, 9].

[1] G. Barcza, Ö. Legeza, K. H. Marti, and M. Reiher, Phys. Rev. A 83, 012508 (2011).
[2] Ö. Legeza, F. Gebhard, and J. Rissler, Phys. Rev. B 74, 195112 (2006).
[3] K. H. Marti, B. Bauer, M. Reiher, M. Troyer, and F. Verstraete, New J. Phys. 12, 103008 (2010).
[4] J. Eisert, M. Cramer, and M. B. Plenio, Rev. Mod. Phys. 82, 277 (2010).
[5] N. Schuch, M. M. Wolf, F. Verstraete, and J. I. Cirac, Phys. Rev. Lett. 100, 030504 (2008).
[6] V. Murg, F. Verstraete, Ö. Legeza, and R. M. Noack, Phys. Rev. B 82, 205105 (2010).
[7] E. Fertitta, B. Paulus, G. Barcza, and Ö. Legeza, arXiv:1406.7038 (2014).
[8] T. Barthel, C. Pineda and J. Eisert, Phys. Rev. A 80, 042333 (2009).
[9] P. Corboz, G. Evenbly, F. Verstraete, and G. Vidal, Phys. Rev. A 81, 010303 (2010).