Density functional theory and tensor product states

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Motivation

- tensor product states (TPS) find their main application in the interplay between quantum information and condensed matter theory
- they are built by restricting the coefficients of the wave function to the contraction of a tensor network.

\[ |\Psi_{TPS}\rangle = \sum_{\alpha_1,\ldots,\alpha_N} F(A_{\alpha_1}^1 \cdots A_{\alpha_N}^N |s_1 \cdots s_N) \]

\( U \) performs the contraction over the tensors \( A_i^\alpha \)

- an example in 2d [1,2]

- their properties make TPS a promising variational family of states for strongly correlated quantum many-body systems

Matrix product states

- matrix product states (MPS) constitute a particular class of 1d TPS
- they represent the variational wave functions that underlie the density matrix renormalization group [3]
- as such they have proven extremely successful in the approximation of ground states, and can also be used for time evolution
- the MPS coefficients comprise a product of matrices \( A_i^\alpha \) for \( 1 \leq i \leq N \) which is surrounded by two vectors \( A_1^\alpha \) and \( A_N^\alpha \)

\[ |\Psi_{MPS}\rangle = \sum_{\alpha_1,\ldots,\alpha_N} A_{\alpha_1}^1 A_{\alpha_2}^2 \cdots A_{\alpha_N}^N |s_1 \cdots s_N \rangle \]

- the MPS tensor network graphically represented:

DFT + MPS

- in order to obtain a lattice problem suited for TPS as in [4], we discretize space such that the external potential \( V = (v_1, v_2, \ldots, v_N) \) and the density \( \tilde{\rho} = (n_1, n_2, \ldots, n_N) \) are evaluated on a grid
- we can construct the non-interacting and interacting Hohenberg-Kohn functionals \( F_{\text{H-K}}^{\text{iso}} \) and \( F_{\text{H-K}}^{\text{iso}} \) from MPS ground state energies:

\[ F_{\text{H-K}}^{\text{iso}} \left( \rho \right) = E^{\text{H-K}}(\rho) - \rho \cdot \int \text{d}^3r \text{d}^3s \rho \cdot \rho \]

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(\( \rho \) denotes the external potential to the density \( \rho \))
- the full Hohenberg-Kohn functional on a grid of \( N \) points can be seen as a tensor of rank \( N \):

Conclusions & Outlook

- the approximation error features a clear exponential decrease with the number of Schmidt coefficients, and thus MPS well approximate the full Hohenberg-Kohn functional of the small Hubbard chains considered here
- when the non-interacting Hohenberg-Kohn functional is subtracted before the approximation, the error improves roughly by one order of magnitude
- in all cases we observe that systems with weak interactions can be better approximated
- we therefore expect that this scheme works worse in case of the long-range interactions of the Coulomb problem: work in progress

Hohenberg-Kohn functional as MPS

- the exact Hohenberg-Kohn tensor is approximated as a MPS via successive truncated singular value decompositions:

\[ \rho_{\text{MPS}}(\mathbf{r},\mathbf{s}) = \sum_{\alpha} \langle \psi_{\alpha} | \mathbf{r} \rangle \psi_{\alpha}^{\dagger} | \mathbf{s} \rangle \]

- the error of the MPS approximation can be read off from the decay of the Schmidt coefficients \( \lambda_{\alpha} \)
- we consider a Hubbard chain:

\[ H = -J \sum_{\langle ij \rangle} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i n_i \]

and compute the Hohenberg-Kohn tensor on a density grid via interacting inversion as in [5,6]; for each desired \( \rho_{\text{MPS}} \) we iteratively adjust \( \mathbf{r} \) according to the obtained \( \rho_{\text{MPS}} \) such that after interaction \( i \) the next \( \mathbf{r} \) reads \( \mathbf{r}_{i+1} = \mathbf{r}_i + \alpha (\mathbf{r}_i - \mathbf{r}_{i-1}) \) with \( \alpha = 0.1 \)

- we investigate 6 fermions on 6 lattice sites and impose a density spacing of 0.3 on each site that ranges from 0.4 to 1.6:

\[ G_{\text{HF}}(\delta) : \text{MPS approximation with D Schmidt coefficients of } F_{\text{H-K}}^{\text{HF}}(\delta) \]

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\[ \omega = \left( \sum_{\alpha} | \lambda_{\alpha} |^2 \right) - \left( \sum_{\alpha} | \lambda_{\alpha} |^2 \right) \]

References