# Supplementary Materials for "Augmenting Density Matrix Renormalization Group with Disentanglers"

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### Optimization of FAMPS

We use a one dimensional representation of FAMPS (as shown in Fig. 1 (c) in the main text) to illustrate the optimization steps. The optimization process of FAMPS is similar as MPS which consists of the calculation of environment tensors and the solving of an eigenvalue problem. The difference is that in FAMPS the calculation of environment is more involved because of the disentangler layer. Here, we consider a Hamiltonian which only contains two-site operators,

$$H = \sum_{ij} h_{ij} \tag{1}$$

We first discuss the optimization of the tensors of MPS. Because disentanglers cannot share the same site, each term of $H$ is mostly connected to two disentanglers. Thus, after the application of disentanglers, any two-site operator $h_{ij}$ connects with at most four sites

$$h'_{ij} = D(u)^\dagger h_{ij} D(u) = u^\dagger_{ik} u^\dagger_{jl} h_{ij} u_{ik} u_{jl} = O_{ijkl} \tag{2}$$

where $D(u) = \prod_m u_m$ represents the disentangler layer. Other disentanglers not acting on sites $i, j$ are annihilated due to $u^\dagger u = I$. The Hamiltonian $H$ becomes

$$H' = D(u)^\dagger \sum_{ij} h_{ij} D(u) = \sum_{ij} h'_{ij} \tag{3}$$

where $h'_{ij}$ is at most a four-site operator. So, a FAMPS with a Hamiltonian $H$ is transformed to an MPS with an effective Hamiltonian $H'$. More specifically,

$$\begin{aligned} \langle \text{FAMPS}|H|\text{FAMPS}\rangle &= \langle \text{MPS}|D(u)^\dagger H D(u)|\text{MPS}\rangle \\ &= \langle \text{MPS}|H'|\text{MPS}\rangle \end{aligned} \tag{4}$$

Thus, we can follow the procedures in MPS to optimize MPS tensors in FAMPS. An environment of an MPS tensor for a four-site operator is shown in Fig. 1 (a). The contraction of it has a cost of $O(D^3)$. We need to calculate the environment for each term in the Hamiltonian $H$ to get the overall environment.

For the optimization of disentanglers, we follow the procedure shown in Ref. [1, 2] where the key step is also the computation of environment. Here, after the application of disentanglers, any two-site operator $h_{ij}$ is also at most a four-site operator

$$h''_{ij} = \prod_m u^\dagger_m h_{ij} \prod_{m \neq \{ik\}} u_m = u^\dagger_{ik} u^\dagger_{jl} h_{ij} u_{jl} = O'_{ijkl} \tag{5}$$

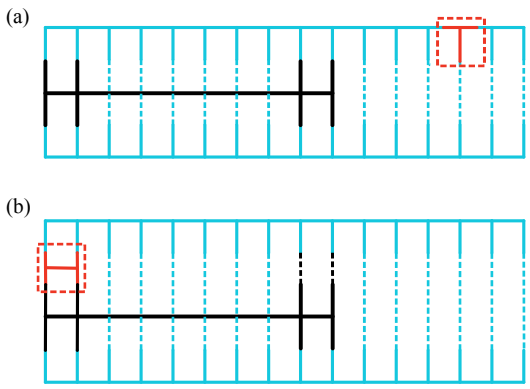


FIG. 1: (a) The environment for an MPS tensor. (b) The environment for a disentangler. The contractions of (a) and (b) can be performed with a computational cost of $O(D^3)$. The black line denotes a four-site operator. The red lines are the tensors to be optimized.

where $u_{ik}$ is the disentangler we want to optimize. Fig. 1 (b) shows the corresponding environment for a disentangler, which can also be contracted with a complexity of $O(D^3)$. The overall environment only involves Hamiltonian terms which are directly attached to the disentangler $u_{ik}$, which makes the optimization of disentanglers very fast. All other Hamiltonian terms contribute a constant term to the energy expectation value and are independent of $u_{ik}$ [1]. More specifically,

$$\begin{aligned} \langle \text{FAMPS}|H|\text{FAMPS}\rangle &= \langle \text{MPS}|D(u)^\dagger H D(u)|\text{MPS}\rangle \\ &= \langle \text{MPS}|\sum_p h''_p u_{ik}|\text{MPS}\rangle + C_{ik} \end{aligned} \tag{6}$$

where $p$ represents the Hamiltonian terms that act on $u_{ik}$ and $C_{ik} = \langle \text{MPS}|\sum_k h'_k|\text{MPS}\rangle$ with $k$ the other Hamiltonian terms not acting on $u_{ik}$.

Overall, the optimization process of FAMPS is divided into two steps: the optimization of disentanglers and the optimization of the MPS tensors. For the optimization of disentanglers, the procedure is described as follows.

(i) select a disentangler $u$, calculate the environments for this disentangler from the Hamiltonian terms that are directly attached to it, add them up to get the overall environment $E$.

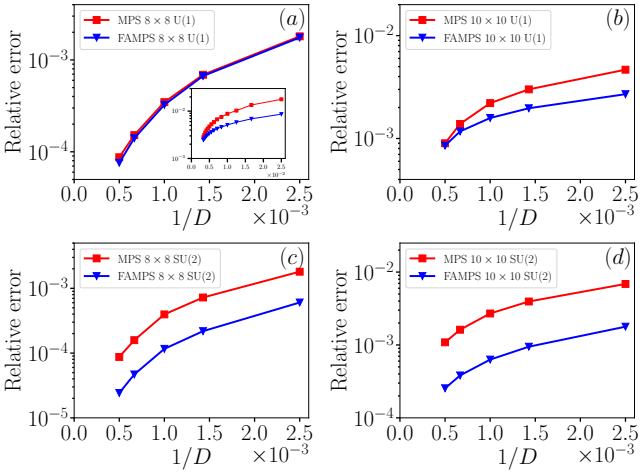


FIG. 2: Relative error of the ground state energy for FAMPS and MPS of the Heisenberg model for lattice sizes $8 \times 8$ and $10 \times 10$ with open boundary conditions. Simulations in (a) and (b) utilize U(1) symmetry and have a physical bond dimension $d = 2$, while in (c) and (d), we use SU(2) symmetry and have a physical bond dimension $d = 4$ by blocking two sites into one site. We can find that by allowing more free parameters in the disentanglers (in (c) and (d)), the critical bond dimension problem (in (a) and (b)) is solved.

(ii) perform a Singular Value Decomposition (SVD) for environment $E = USV^\dagger$, then calculate the optimized disentangler $u_{\text{new}} = -VU^\dagger$.

(iii) move to another disentangler and repeat (i) and (ii) until all the disentangles are optimized once.

After optimizing the disentanglers for $3 \sim 5$ sweeps, we move to the optimization of MPS tensors. The optimization of MPS tensors follows the below steps.

(i) choose an MPS tensor $T$, set the tensor $T$ as the center tensor as in MPS optimization algorithm.

(ii) calculate the environments for this tensor $T$ from all the Hamiltonian terms and add them up to get the overall environment.

(iii) use the Lanczos or similar algorithm to solve the eigenvalue problem for tensor T. In this step, step (ii) needs to be repeated for several times.

(iv) move to a next MPS tensor and repeat step (i), (ii) and (iii) until all the MPS tensors are optimized.

Then, we repeat the process by optimizing disentanglers and MPS tensors alternatively until the energy is converged.

### Critical Bond Dimension in FAMPS

As mentioned in the main text, in the study of Heisenberg model with open boundary conditions we encounter the problem of critical bond dimension in FAMPS. The results are shown in Fig. 2. In (a) and (b), we can find that with the increase of bond dimension, there exist a critical bond dimension after which the results of FAMPS and MPS are identical. This phenomenon is related to the absence of free parameters of disentanglers. For spin 1/2 degree of freedom, each site has physical dimension $d = 2$ and can be labeled by quantum number $\{0, 1\}$. Under U(1) symmetry, disentangler $u_{ij}^{kl}$ can be written as (we only consider real entries for $u_{ij}^{kl}$)

$$u_{ij}^{kl} = u_0 \oplus u_1 \oplus u_2 \tag{7}$$

where $u_1$ is a $2 \times 2$ matrix and $u_0, u_2$ are $1 \times 1$ matrices or numbers. Due to the unitary property of disentangler, $u_0^2 = 1, u_2^2 = 1, u_1^\dagger u_1 = I_{2\times 2}$. Thus, disentangler $u_{ij}^{kl}$ can be written as

$$u_{ij}^{kl} = \pm 1 \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \sin\theta & \cos\theta & 0 \\ 0 & -\cos\theta & \sin\theta & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{8}$$

Thus, disentangler $u_{ij}^{kl}$ has only one free parameter under U(1) symmetry. But under SU(2) symmetry, disentangler $u_{ij}^{kl}$ is written as (using the notation in Ref. [3])

$$u_{ij}^{kl} = (P_0 \otimes Q^0_{\frac{1}{2},\frac{1}{2}\to\frac{1}{2},\frac{1}{2}}) + (P_1 \otimes Q^1_{\frac{1}{2},\frac{1}{2}\to\frac{1}{2},\frac{1}{2}}) \tag{9}$$

where $P_0, P_1$ are numbers, $Q^0_{\frac{1}{2},\frac{1}{2}\to\frac{1}{2},\frac{1}{2}}$ and $Q^1_{\frac{1}{2},\frac{1}{2}\to\frac{1}{2},\frac{1}{2}}$ are matrix determined by Clesch-Gordan coefficients, which are $\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1/2 & -1/2 & 0 \\ 0 & -1/2 & 1/2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$ and $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1/2 & 1/2 & 0 \\ 0 & 1/2 & 1/2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$ respectively. Under the restriction of $u^\dagger u = I$, $P_0^2 = P_1^2 = 1$, which leads to $P_0 = \pm 1, P_1 = \pm 1$. Thus, disentangler $u_{ij}^{kl}$ has no free parameter under SU(2) symmetry. When considering Z(2) symmetry (in the transverse Ising

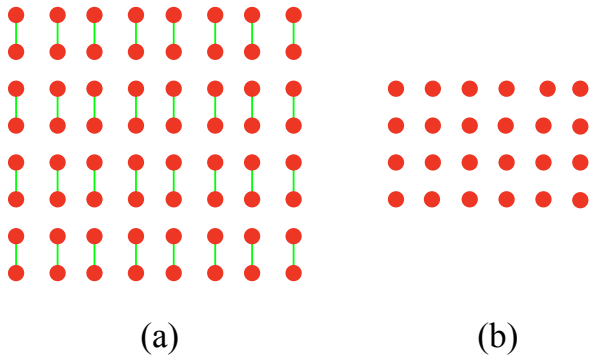


FIG. 3: To increase the number of free parameters in disentanglers for the Heisenberg model, we block two sites linked by green lines in (a) into one site.

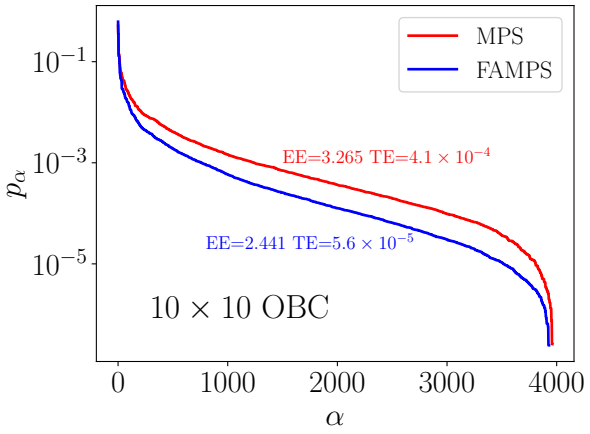


FIG. 4: The distribution of the entanglement spectrum for the Heisenberg model on a $10 \times 10$ lattice under open boundary conditions. The bond dimension for both MPS and FAMPS are $D = 1000$. The result for the FAMPS is for the underlying MPS (without disentanglers). We can see that both the entanglement entropy (EE) and truncation error (TE) are reduced in FAMPS.

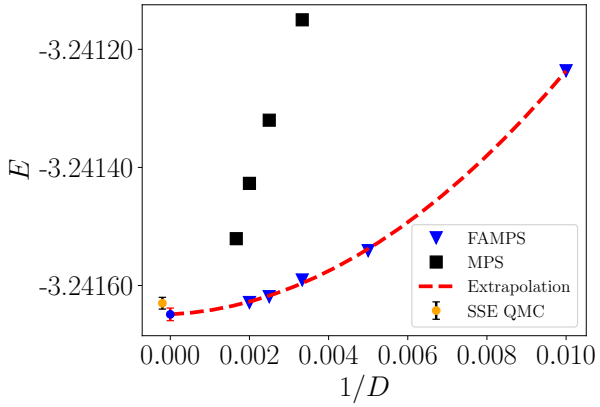


FIG. 5: A quadratic extrapolation of the FAMPS energy per site of a $8 \times 8$ transverse Ising model with $\lambda = 3.05$ under periodic boundary conditions. The fit gives an extrapolated value of ground state energy per site $E = -3.24165(1)$ which agrees with the SSE QMC result $-3.24163(1)$ within the error bar.

model), disentangler $u_{ij}^{kl}$ can be written as

$$u_{ij}^{kl} = u_0 \oplus u_1 \tag{10}$$

where $u_0$, $u_1$ are $2 \times 2$ matrix satisfying $u_1^\dagger u_1 = u_2^\dagger u_2 = I_{2\times 2}$. Then, disentangler $u_{ij}^{kl}$ can be represented as

$$u_{ij}^{kl} = \begin{pmatrix} \sin\alpha & 0 & 0 & \cos\alpha \\ 0 & \sin\beta & \cos\beta & 0 \\ 0 & -\cos\beta & \sin\beta & 0 \\ -\cos\alpha & 0 & 0 & \sin\alpha \end{pmatrix} \tag{11}$$

Here, disentangler $u_{ij}^{kl}$ has two free parameters. Thus, in Transverse Ising model, there is no critical bond dimension as shown in Fig. 2 in the main text.

For the U(1) symmetry imposed DMRG calculations in Fig. 2 (a) and (b), SU(2) symmetry is nearly restored after the critical bond dimension, which means the disentanglers have no free parameter and FAMPS results are identical to MPS ones. To solve this problem, we can block two sites into one to enlarge the physical degrees of freedom as shown in Fig. 3. In this way, we increase the number of free parameters in the disentanglers. Fig. 2 (c) and (d) show calculations with the same models in Fig. 2 (a) and (b). From Fig. 2, we can find that the FAMPS results are always better than MPS results and there is no critical bond dimension.

### Comparison of the entanglement spectrum

In Fig. 4, we show the the distribution of the entanglement spectrum for the Heisenberg model on a $10 \times 10$ lattice under open boundary conditions. The bond dimension for both MPS and FAMPS are $D = 1000$. The result for the FAMPS is for the underlying MPS (without disentanglers). We can see that both the entanglement entropy (EE) and truncation error (TE) are reduced in FAMPS, which demonstrates the effect of disentanglers to reduce the entanglement in the ground state wavefunction and hence to increase the accuracy of MPS.

### More Results

In Fig. 5, we show the extrapolation of FAMPS energy with bond dimension for the transverse Ising model with periodic boundary conditions and $\lambda = 3.05$ on a $8 \times 8$ lattice. A quadratic fit gives the extrapolated value of ground state energy per site $E = -3.24165(1)$ which agrees with the SSE QMC result $-3.24163(1)$ within the error bar.

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[1] G. Evenbly and G. Vidal, Phys. Rev. B **79**, 144108 (2009), URL https://link.aps.org/doi/10.1103/PhysRevB.79.144108.

[2] T. Felser, S. Notarnicola, and S. Montangero, Phys. Rev. Lett. **126**, 170603 (2021), URL https://link.aps.org/doi/10.1103/PhysRevLett.126.170603.

[3] S. Singh and G. Vidal, Phys. Rev. B **86**, 195114 (2012), URL https://link.aps.org/doi/10.1103/PhysRevB.86.195114.