1 MPS-based Lanczos method

As discussed during the lecture course, the Lanczos method is an efficient way to find the eigenvectors of a large Hermitian matrix. It can be generalized by using MPSs as vectors and an MPO as the matrix. This generalization idea is proposed in Ref. 1. In this exam topic, you are asked to implement this idea and to test it.

(a) Read the "Method" part of Ref. 1 and write your code for the MPS-based Lanczos method. What is the difference between the ordinary Lanczos method and this MPS-based method? Note that, in Ref. 1, $|\psi_i\rangle$'s and $|\Psi_i\rangle$'s indicate different types of states.

(b) Reproduce Fig. 1 of Ref. 1, i.e., use the MPS-based Lanczos method to compute the ground-state energy and the entanglement entropy of the spin-1/2 Heisenberg chain with $N = 20$ spins.

(c) Increase the system size N and try your best to reproduce some results in Fig. 2 of Ref. 1. Compare with the DMRG (two-site or controlled bond expansion) results.

References

[1] R.-Z. Huang, H.-J. Liao, Z.-Y. Liu, H.-D. Xie, Z.-Y. Xie, H.-H. Zhao, J. Chen, and T. Xiang, arXiv:1611.09574 (2016).

2 Infinite-size DMRG

The goal of this problem is to implement the infinite-size DMRG (iDMRG) for the anti-ferromagnetic $S = 1/2$ Heisenberg chain with open boundary conditions,

$$\hat{H}_{\text{Heisenberg}} = \sum_{\langle ij \rangle} \left[\hat{S}_i^z \hat{S}_j^z + \frac{1}{2}(\hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+) \right],$$

and the Ising model in a transverse field with open boundary conditions,

$$\hat{H}_{\text{Ising}} = \sum_{\langle ij \rangle} \hat{S}_i^z \hat{S}_j^z + \lambda \sum_i \hat{S}_i^x,$$

where $\hat{S}_i^\alpha$ are local spin-1/2 operators on site i. Here we refer to the figures and equations of Ref. 1.

(a) Implement the iDMRG for translation invariant systems of a two-site unit cell. The procedure is summarized in Fig. 1.

(b) Benchmark your implementation by computing the ground state energy per site for the Heisenberg model and compare with the exact result for an infinite chain $e_0 = (1/4) - \ln(2)$ [2]. The energy per site e_0 can be extracted from the difference between total energies E_0 for two consecutive iDMRG iteration, $e_0(N) = [E_0(N) - E_0(N-2)]/2$. Check your results with different bond dimensions $D = 20, 30, 40, 50$. (With $D = 40$ or 50, you would be able to achieve decent accuracy in energy $\approx 10^{-4}$ or 10^{-5}, respectively.)

(c) Verify the claim in Ref. 1 that the trial wave function used in the step 4 of Fig. 1 is a good choice, by computing the fidelity $1 - \langle \Psi_n^{\text{trial}} | \Psi_n \rangle$. Make a plot similar to Fig. 2 for the Heisenberg model.

(d) Analyze the behavior of iDMRG for the Ising model at the critical point $\lambda = 1/2$ by studying the spectrum of the transfer operator [see Eq. (28)]. Make a plot similar to Fig. 4.

References

[1] I. P. McCulloch, arXiv:0804.2509 (2008).

[2] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).

3 Variational uniform MPS

The goal of this problem is to implement the variational uniform MPS (VUMPS) algorithm introduced in Ref. 1 and use it to compute properties of the ferromagnetic transverse-field Ising (TFI) model. A useful review of the uniform MPS (uMPS) is provided in Ref. 2. An analytic solution to the TFI model can be found from Ref. 3. The TFI model Hamiltonian is given by

$$\hat{H}_{\mathrm{TFI}} = -\sum_i \hat{S}^z - 2\lambda \sum_i \hat{S}^x_i \hat{S}^x_{i+1} \,,$$

where λ is a tuning parameter and $\hat{S}^\alpha_i$ are local spin-1/2 operators.

(a) Implement the VUMPS method for the translation invariant systems with a one-site unit cell. We recommend to proceed as follows, though it's ultimately up to you to come up with a working code. Here we refer to Ref. 1 for sections, figures, and equations, unless specified.

- Implement the algorithm as described in Secs. II A–II D.
- To initialize a uMPS, it is helpful to implement the algorithm that brings a uMPS from the uniform gauge to the mixed canonical gauge as described in Sec. II A. Step-by-step details can be found from Sec. 2.3 of Ref. 2. Here, you will need to implement the Arnoldi algorithm to find the dominant left and right eigenvectors of a transfer matrix. The Arnoldi algorithm is similar to the Lanczos algorithm, but also works for non-Hermitian matrices. Refer to, e.g., the Wikipedia entry [4] for the details of the algorithm.
- Find the effective Hamiltonian, following the recipe described in Sec. II B and Table I. The construction of some terms involves geometric sums of transfer matrices, which is explained in App. D. Note that we recommend the `gmres` function of MATLAB to solve Eq. (D13).
- Obtain the ground state by using the iterative update procedure described in Sec. II C. We recommend to update MPS tensors via the QR decomposition [see Eq. (21)].

(b) After implementing the VUMPS algorithm, apply it to the *ferromagnetic* TFI model, defined by $\hat{H}_{\mathrm{TFI}}$ above. (Quick question: why would VUMPS with one-site unit cell not work for the *antiferromagnetic* models?) Using $D = 40$ and $\lambda \in \{0.9, 1.1\}$, show how the VUMPS results of the ground-state energy density E_0/N, the magnetization $\langle \hat{S}^z_i \rangle$, and a correlation function $\rho^x_\infty = \lim_{n\to\infty} \langle \hat{S}^x_i \hat{S}^x_{i+n} \rangle$ approach the analytical results [3] as a function of iteration number. What are your best results in terms of the smallest errors? Also show how the gradient norm $||B||$ approaches zero as a function of iteration number, similarly to Fig. 1 in Ref. 1.

(c) Compute E_0/N, $\langle \hat{S}^z_i \rangle$ and ρ^x_∞ as a function of λ across $\lambda = 1$ and compare your numerical result to the analytic expressions in Ref. 3.

(d) At $\lambda = 1$, one finds $\rho^z_n = \langle \hat{S}^z_i \hat{S}^z_{i+n} \rangle - \langle \hat{S}^z_i \rangle^2 = [\pi^2(4n^2-1)]^{-1}$. Depending on the bond dimension D, how well and up to what value of n can you reproduce this result? Comment on possible qualitative deviations of the VUMPS results compared to the exact formula and how these change with D. Consider also very low values of D, e.g., $D = 2$, but also try to push D to very large values, depending on what your computer can handle.

References

[1] V. Zauner-Stauber, L. Vanderstraeten, M. T. Fishman, F. Verstraete, and J. Haegeman, Phys. Rev. B **97**, 045145 (2018).

[2] L. Vanderstraeten, J. Haegeman, and F. Verstraete, SciPost Phys. Lect. Notes **7** (2019).

[3] P. Pfeuty, Ann. Phys. **57**, 79 (1970).

[4] Wikipedia: Arnoldi iteration.

4 Tensor network representations of parton wave functions

Parton wave functions, such as projected Fermi sea states, are useful variational ansätze for the ground states of many strongly correlated systems. The Fermi sea, the ground state of some non-interacting parton Hamiltonian, is given by $\prod_{\epsilon_k<0} \hat{d}_k^\dagger |0\rangle$, where $\hat{d}_k^\dagger$ creates a particle at the single-particle eigenmode of energy ϵ_k, and $|0\rangle$ is the fermionic vacuum. Then the so-called Gutzwiller projection is applied to the sea state.

In this problem set, we follow the method, proposed in Ref. 1, that obtains the MPS representation of parton wave functions. We first construct the half-filled Fermi sea for spin-1/2 systems. Then we apply the Gutzwiller projector to project each lattice site onto the singly-occupied state. Here we refer to Ref. 1 for figures and equations, unless specified.

(a) Construct the half-filled Fermi sea for the Haldane-Shastry model of length $N = 32$. As shown in Eq. (2), the creation operators for single-particle orbitals can be represented as matrix product operators (MPO) of $D = 2$. Construct the MPS for the half-filled Fermi sea by sequentially applying the MPO for $d_k^\dagger$ to the MPS, starting from the vacuum state. Details can be found from Sec. I of the Supplemental Material of Ref. 1 and Sec. III of Ref. 2. Plot the entanglement entropy at the center of the system versus the number of applied single-particle eigenmodes with a maximal bond dimension cutoff, $D_{\max} = 100$. Your result should look similar to the red line in Fig. 2(b).

(b) Construct the maximally localized Wannier orbitals for the occupied single-particle eigenmodes, following the paragraph *Compressing into MPS*. Plot the entanglement entropy at the center of the system versus the number of applied Wannier orbitals from left to right with a maximal bond dimension cutoff, $D_{\max} = 100$. Your result should look similar to the blue line in Fig. 2(b).

(c) Similarly to the problem (c), plot the entanglement entropy at the center of the system versus the number of applied Wannier orbitals, but now with the left-meet-right strategy. Your result should look similar to the magenta line in Fig. 2(b).

(d) Apply the Gutzwiller projection and compute the energy and the spin-spin correlation functions with respect to the projected wave function. Compare your result with the exact results given in Eq. (7) and Table I.

References

[1] Y.-H. Wu, L. Wang, and H.-H. Tu, Phys. Rev. Lett. **124**, 246401 (2020).

[2] H.-K. Jin, H.-H. Tu, and Y. Zhou, Phys. Rev. B **101**, 165135 (2020).

5 XTRG

The exponential tensor renormalization group (XTRG) [1] is one of the most robust methods to compute the thermal density matrix $\rho = e^{-\beta H}$ for finite-size quantum systems, where β is the inverse temperature and H is the moany-body Hamiltonian. We will compute the partition function of a one-dimensional XY model using XTRG proceed from the high-temperature limit $\beta \sim 10^{-6}$ down to the low temperatures $\beta \sim 1$.

(a) Initialize the density matrix as an MPO by using linear initialization $\rho(\beta) \approx 1 - \beta H$, as described in Appendix C.2 of Ref. [1].

(b) Develop an XTRG code, following the methodology described in Sec. II of Ref. [1]. The key idea is as follows: given the density matrix $\rho(\beta)$ at some inverse temperature β, one can obtain the density matrix $\rho(2\beta)$ at a lower temperature by exploiting the identity $\rho(2\beta) = \rho(\beta) \times \rho(\beta)$, i.e. by multiplying the MPO $\rho(\beta)$ with itself. This operation inevitably increases the bond dimension, necessitating a truncation. This can be done variationally using DMRG-type sweeping (see Appendix D of Ref. [1]).

(c) Compute the thermal density matrix of a one-dimensional XY model of length $L = 10$. Start from $\beta_0 = 10^{-6}$, and run 20 XTRG iterations to reach the low temperature phase at $\beta = 2^{20}\beta_0$. Compute the partition functions and compare your result with the analytical solution given in Appendix F of Ref. [1], for all temperature values covered.

References

[1] B.-B. Chen, L. Chen, Z. Chen, W. Li, and A. Weichselbaum Phys. Rev. X **8**, 031082 (2018).