1 Single-site excitation Ansatz

The excitation Ansatz is a tensor network that constructs excited states on top of a ground-state MPS. In this problem, you will implement the single-site excitation Ansatz to compute the lowest-energy excited state of a one-dimensional free-fermion model with pairing terms:

$$\mathcal{H}_{\mathrm{ff}} = -\frac{1}{2}\sum_{\ell}^{\mathscr{L}-1}\left[(c_\ell^\dagger c_{\ell+1} + c_\ell^\dagger c_\ell + 1) + \gamma(c_\ell^\dagger c_{\ell+1}^\dagger + c_\ell c_{\ell+1})\right] . \tag{1}$$

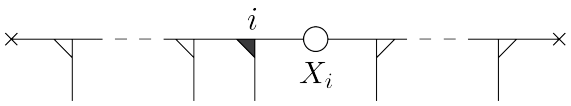
Using a Jordan-Wigner transformation, this Hamiltonian maps to the anisotropic spin-1/2 XY model:

$$\mathcal{H}_{\mathrm{XY}} = \sum_{\ell}^{\mathscr{L}-1}\left[(1+\gamma)S_\ell^x S_{\ell+1}^x + (1-\gamma)S_\ell^y S_{\ell+1}^y\right] . \tag{2}$$

Analytically, the presence of pairing in the fermionic Hamiltonian induces an energy gap $\Delta = \gamma$, defined as the difference between the lowest excitation energy and the ground-state energy.

(a) Implement the MPO representations for $\mathcal{H}_{\mathrm{ff}}$ and $\mathcal{H}_{\mathrm{XY}}$. Use DMRG to obtain the ground-state MPS for both models. Verify that the ground-state energies agree up to numerical precision (difference $< 10^{-8}$).

(b) The quasiparticle Ansatz in Sec. II of Ref. [1] corresponds to the single-site excitation ansatz (i.e., $n = 1$) described in Sec. V of Ref. [2]. Rewrite the Ansatz in Sec. II of Ref. [1] using the kept/discarded space language and show that it is orthogonal to the ground state. Your result should resemble the diagram below:

$|\Phi(X_i)\rangle = \sum_i$ 

(c) Derive the procedure for applying the Hamiltonian to the excitation Ansatz using the kept/discarded space language, based on the Appendix of Ref. [1]. Note that Eqs. (A3) (right) and (A7) (second term) in Ref. [1] are incorrect. Derive the correct expressions using Eqs. (79a) and (79b) from Sec. V of Ref. [2].

(d) Implement both the single-site excitation Ansatz and the application of the Hamiltonian to the Ansatz.

(e) Use the Lanczos eigensolver to compute the lowest excitation energy of $\mathcal{H}_{\mathrm{ff}}$. Plot the energy gap Δ as a function of system size $\mathscr{L}$, starting from $\mathscr{L} = 50$ and increasing as far as your resources allow. Verify that the computed energy gap converges to γ as $\mathscr{L}$ increases.

(f) Fix $\mathscr{L} = 50$ and bond dimension $D = 50$. Gradually decrease γ from 0.3 to 0.001 and monitor the energy gap. What happens as γ becomes small? (*Hint:* Consider the roles of the finite-size effects and bond dimension limitations.)

Tips for implementation:

(i) Start with $\mathscr{L} = 50$, $D = 50$, and $\gamma = 0.3$. Run at least 100 Lanczos iterations. At these parameters, the energy gap deviation should be $\mathcal{O}(10^{-3})$.

(ii) The Lanczos algorithm should return eigenvectors,which are useful for debugging.

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2 Infinite-size DMRG

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

$$H = \sum_{\langle ij \rangle} \left[\frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+) + S_i^z S_j^z \right],$$

and the transverse-field Ising (TFI) chain with open boundary conditions,

$$H = \sum_{\langle ij \rangle} S_i^z S_j^z + \lambda \sum_i S_i^x,$$

where S_i^α are local spin-1/2 operators on site i.

(a) Implement the iDMRG for a translation-invariant system of a two-site unit cell. The procedure is outlined in Fig. 1 of Ref. [1].

(b) Benchmark your implementation by computing the ground-state energy per site for the Heisenberg chain, and compare it with the exact result in the thermodynamic limit $e_0 = \frac{1}{4} - \ln 2$ [2].

To estimate e_0, use the difference in total energies of two consecutive iDMRG iterations, $e_0(N) = \frac{E_0(N) - E_0(N-2)}{2}$. Run simulations with different bond dimensions $D = 20, 30, 40, 50$.

Hint: With $D = 50$ (resp. $D = 20$), you should be able to obtain ground-state energies accurate to within 10^{-5} (resp. 10^{-4}).

(c) In step 4 of Fig. 1 in Ref. [1], a specific trial wave function is used to initialize the next iteration. Verify that this choice is effective by computing the fidelity loss $1 - \langle \Psi_n^{\text{trial}} | \Psi_n \rangle$. Generate a plot similar to Fig. 2 in Ref. [1], using the Heisenberg chain.

(d) Study the behavior of iDMRG using the TFI chain at its critical point, $\lambda = 1/2$. Analyze the spectrum of the transfer operator (see Eq. (28) in Ref. [1]) and generate a plot similar to Fig. 4 in Ref. [1].

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3 Variational uniform MPS

The goal of this problem is to implement the variational uniform MPS (VUMPS) algorithm, as introduced in Ref. [1], and use it to compute ground-state properties of the ferromagnetic transverse field Ising (TFI) chain. A useful pedagogical reference on uniform MPS (uMPS) is Ref. [2]. The exact solution of the TFI chain can be found in Ref. [3]. The model Hamiltonian is given by

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

where λ is a tuning parameter and S^α_i are spin 1/2 operators on site i.

(a) Implement the VUMPS algorithm for translation-invariant systems with a 1-site unit cell. We recommend the following steps:

- Implement the main VUMPS iteration as described in Secs. II A–D of Ref. [1].
- To initialize the uMPS, implement the procedure for converting a uMPS in uniform gauge to mixed canonical gauge, as described in Sec. II A of Ref. [1]. Step-by-step details can be found in Sec. 2.3 of Ref. [2]. This step requires computing dominant left/right eigenvectors of a transfer matrix, for which you should implement the Arnoldi algorithm — a generalization of the Lanczos method for non-Hermitian matrices. For reference, see the Wikipedia entry [4].
- Construct the effective Hamiltonian as described in Sec. II B of Ref. [1]. Pseudocode is given in Table I. The construction of some terms involves geometric sums of transfer matrices. Some terms involve geometric series of transfer matrices, discussed in Appendix D of Ref. [1]. To solve Eq. (D13) in Ref. [1], we may use the GMRES algorithm (Julia package available; see Ref. [5]).
- To minimize the energy and update the MPS tensor, follow the iterative procedure described in Sec. II C of Ref. [1]. We recommend the method based on QR decomposition, as used in Eq. (21) of Ref. [1].

(b) Apply your implementation to the ferromagnetic TFI model defined above. (*Quick question:* Why would VUMPS with 1-site unit cell not work for the antiferromagnetic TFI chain?). Using $D = 40$ and $\lambda \in \{0.9, 1.1\}$, show how ground-state energy density $\frac{E_0}{N}$, $\langle S^z_i\rangle$ and $\rho^x_\infty = \lim_{n\to\infty}\langle S^x_i S^x_{i+n}\rangle$ computed with VUMPS approach the analytical result as a function of iteration number. How small is the error you are able to achieve? Also show how the norm of the gradient $|B|$ approaches zero as a function of iteration number, similar to Fig. 1 in Ref. [1]. For the analytical expressions, see Ref. [3].

(c) Compute $\frac{E_0}{N}$, $\langle S^z_i\rangle$, and ρ^x_∞ as a function of λ across the critical point $\lambda = 1$ and compare your numerical results with the analytical expressions in Ref. [3].

(d) At the critical point $\lambda = 1$, the connected spin–spin correlation function has the exact form $\rho^z_n = \langle S^z_i S^z_{i+n}\rangle - \langle S^z_i\rangle^2 = \frac{1}{\pi^2(4n^2-1)}$. Depending on the bond dimension D, how well and up to what value of n can you reproduce this result? Discuss how the qualitative agreement changes with increasing D. Consider both small D values (e.g., $D = 2$) and large values (e.g., $D = 100$ or more, depending on available memory and runtime).

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4 MPS-based Lanczos method

As discussed in the lectures, the Lanczos method is an efficient iterative algorithm for finding eigenvalues and eigenvectors of large Hermitian matrices. This method can be generalized to variational representations of quantum states, in particular MPS as vectors and MPO as matrices. This generalization was proposed in Ref. [1], where the standard Lanczos procedure is adapted to the MPS–MPO formalism. In this exercise, you will implement this method and benchmark its performance.

(a) Read the "Method" section of Ref. [1] carefully and implement the MPS-based Lanczos algorithm. Explain the key differences between the standard Lanczos method and its MPS-based variant. Note that, in Ref. [1], $|\psi_i\rangle$ and $|\Psi_i\rangle$ indicate different types of states.

(b) Reproduce Fig. 1 of Ref. [1]: Use your MPS-based Lanczos implementation to compute the ground-state energy and the entanglement entropy for the spin-1/2 Heisenberg chain with $N = 20$ spins and open boundary conditions.

(c) Increase the system size N (as far as your computational resources allow), and try to reproduce some of the data shown in Fig. 2 of Ref. [1]. Compare your results with those obtained using the standard two-site DMRG method.

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5 Minimally entangled typical thermal state

The goal of this problem is to implement the minimally entangled typical thermal state (METTS) algorithm for the antiferromagnetic $S = 1$ Heisenberg chain with open boundary conditions:

$$H = \sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z),$$

where S_i^α are spin-1 operators at site i. The METTS algorithm consists of three parts:

(i) Imaginary-time evolution of a classical product state (CPS) $|i\rangle$ to generate a METTS $|\phi(i)\rangle$.

(ii) Collapse of $|\phi(i)\rangle$ into a new CPS $|j\rangle$.

(iii) Sampling and measurement of observables from an ensemble of METTS $\{|\phi(i)\rangle, i = 1, \dots M\}$, obtained by repeating steps (i) and (ii) M times. Expectation values of observables can be estimated using importance sampling:

$$\langle O\rangle = \mathrm{Tr}[\rho O] \approx \frac{1}{M}\sum_i \langle\phi(i)| O |\phi(i)\rangle \ ,$$

where O is an operator and $\rho \propto e^{-\beta H}$ is the thermal density matrix.

(a) Implement the imaginary-time evolution of product states using time-dependent DMRG (tDMRG) to generate METTS (see Eq. (3) and Sec. 2.1.1 of Ref. [1]).

(b) Implement the CPS collapse algorithm (see Sec. 2.3 of Ref. [1]). Note that after the collapse, the resulting MPS should have $D = 1$.

(c) Efficient sampling requires choosing an appropriate spin basis for the CPS at each step. If you always collapse into the S^z basis, the algorithm may converge slowly. By alternating between S^z and S^x base, one can improve ergodicity. Verify this strategy by reproducing Fig. 6 of Ref. [1].

(d) Compute the magnetic susceptibility $\chi = \frac{\langle {S^z_{\mathrm{tot}}}^2\rangle - \langle S^z_{\mathrm{tot}}\rangle^2}{TN}$ for a chain of $N = 100$ sites at temperatures $T = 0.5, 0.4, 0.3, 0.2, 0.1$. Compare your results to Fig. 1(a) of Ref. [1].

(e) Compute the specific heat $C = \frac{\langle H^2\rangle - \langle H\rangle^2}{TN}$ for the same chain and temperatures as in (d). Compare your results with Fig. 1(b) of Ref. [1].

Note: You may either express H^2 as a sum of local terms or represent H as an MPO so that H^2 is a product of two MPOs.

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6 Tensor network representations of parton wave functions

Parton wave functions, such as projected Fermi sea states, can be efficiently converted into matrix product states (MPSs). The Fermi sea, being the ground state of a non-interacting fermionic Hamiltonian, takes the form $\prod_{\epsilon_k<0} d_k^\dagger |0\rangle$, where $d_k^\dagger$ creates a fermion in the single-particle orbital of energy ϵ_k, and $|0\rangle$ is the fermionic vacuum. To incorporate many-body correlations, one applies the "Gutzwiller projector", which, for spin-1/2 systems, projects each site of a half-filled Fermi sea to the singly occupied subspace. The implementation details are provided in Ref. [1].

(a) Construct the half-filled Fermi sea for the Haldane-Shastry model with chain length $N = 32$. The single-particle orbitals $d_k^\dagger$ are defined in Eq. (6) of Ref. [1]. As shown in Eq. (2), these orbitals can be written as MPOs with bond dimension $D = 2$.

Starting from the fermionic vacuum state, sequentially apply the MPOs $d_k^\dagger$ to form the half-filled Fermi sea as MPS. Implementation details are provided in Supplemental Material (Sec. I) of Ref. [1]. Plot the entanglement entropy at the center of the chain versus the number of applied single-particle eigenmodes using a maximal bond dimension cutoff $D_{\max} = 100$. Your result should resemble the red curve in Fig. 2(b) of Ref. [1].

(b) Construct the maximally localized Wannier orbitals for the occupied single-particle eigenmodes in Eq. (6) of Ref. [1]. The method is described in the section "Compressing into MPS" in the main text.

Apply the Wannier orbitals one by one (ordered from left to right). Plot the entanglement entropy at the center of the chain versus the number of applied Wannier orbitals, using the same bond dimension cutoff $D_{\max} = 100$. Your result should resemble the blue curve in Fig. 2(b) of Ref. [1].

(c) Repeat the calculation of part (b), but apply the Wannier orbitals using the left-meets-right strategy described in Ref. [1]. Compare your results with the magenta curve in Fig. 2(b) of Ref. [1].

(d) After constructing the Fermi sea as an MPS, apply the Gutzwiller projection to enforce single-occupancy on each site. Compute the ground-state energy and spin-spin correlation function. Compare your results with the exact analytical results for the Haldane-Shastry model, which are provided in Ref. [1].

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7 XTRG

The Exponential Tensor Renormalization Group (XTRG) [1] is a powerful numerical method for computing the thermal density matrix $\rho = e^{-\beta H}$ of finite-size quantum systems, where β is the inverse temperature and H is the many-body Hamiltonian. In this problem, you will implement the XTRG algorithm and use it to compute the partition function of a one-dimensional (1D) XY model from high temperatures ($\beta \sim 10^{-6}$) down to low temperatures ($\beta \sim 1$).

(a) Initialize the thermal density matrix as a matrix product operator (MPO) using linear initialization, $\rho(\beta_0) \approx 1 - \beta_0 H$, as described in Appendix C.2 of Ref. [1]. Use $\beta_0 = 10^{-6}$ as the initial inverse temperature.

(b) Implement the XTRG algorithm following the strategy in Sec. II of Ref.[1]. The key idea is to iteratively double the inverse temperature, $\rho(2\beta) = \rho(\beta) \times \rho(\beta)$, by contracting the MPO with itself. After each multiplication, the MPO bond dimension increases and must be truncated. This can be done variationally using DMRG-type sweeping, as detailed in Appendix D of Ref. [1].

(c) Apply your XTRG implementation to the 1D XY model of length $L = 10$. Perform 20 XTRG steps starting from $\beta_0 = 10^{-6}$, so that the final inverse temperature is $\beta = 2^{20}\beta_0$. At each step, compute the partition function $Z = \mathrm{Tr}(\rho(\beta))$. Compare your numerical results with the analytical solution provided in Appendix F of Ref. [1] over the full temperature range.

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8 Crosscap overlap and the Luttinger parameter

The Luttinger parameter is a fundamental quantity that characterizes the low-energy behavior of one-dimensional quantum systems described by Tomonaga–Luttinger liquid theory. In this problem, you will implement the crosscap overlap approach [1] using the DMRG method to extract the Luttinger parameter K from the ground states of critical spin chains. Specifically, you will study two models: the spin-1/2 XXZ chain

$$H_{\mathrm{XXZ}} = \sum_{j=1}^{N} \left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z \right) ,$$

and the spin-1/2 J_1-J_2 Heisenberg chain

$$H_{J_1-J_2} = \sum_{j=1}^{N} (J_1 \mathbf{S}_j \cdot \mathbf{S}_{j+1} + J_2 \mathbf{S}_j \cdot \mathbf{S}_{j+2}) .$$

Note: *Periodic* boundary conditions are imposed in both models. The crosscap state is defined in Eq. (14) of Ref. [1], and the crosscap overlap is defined by $|\langle \mathcal{C}_{\mathrm{latt}} | \Psi \rangle|$, where $|\Psi\rangle$ is the ground state.

(a) Construct MPOs represention for the two Hamiltonians above. *Hint:* For periodic boundary conditions, the Hamiltonian MPO should include the boundary interaction terms. For the XXZ chain, this means adding the term $S_N^x S_1^x + S_N^y S_1^y + \Delta S_N^z S_1^z$. For the J_1-J_2 chain, the boundary terms are $J_1 \mathbf{S}_N \cdot \mathbf{S}_1 + J_2 \mathbf{S}_{N-1} \cdot \mathbf{S}_1 + J_2 \mathbf{S}_N \cdot \mathbf{S}_2$. In practice, for the J_1-J_2 chain, you may construct two MPOs separately (one for the J_1 terms and one for the J_2 terms) and then sum them to form a single MPO with larger bond dimension.

(b) Use DMRG to obtain the ground-state MPS $|\Psi\rangle$ of the spin-1/2 XXZ chain with $N = 100$ sites and varying anisotropy $\Delta \in [-0.9, 1.0]$. Compute the crosscap overlap by contracting the tensor network in Fig. 1(b) of Ref. [1]. Think carefully about how to perform the contraction efficiently. (*Hint:* Fold the chain so that tensors at sites j and $j + N/2$ are paired.) Compare your numerical results with the analytical prediction

$$|\langle \mathcal{C}_{\mathrm{latt}} | \Psi \rangle|^2 = \frac{1}{\sqrt{K}}, \quad K = \frac{\pi}{2(\pi - \arccos \Delta)}, \quad \text{for } \Delta \in (-1, 1)$$

Your result should resemble Fig. 2(a) in Ref. [1].

(c) At the Heisenberg point ($\Delta = 1$), the extracted Luttinger parameter for $N = 100$ shows a clear deviation from the expected value $K = 1/2$. As discussed in Ref. [1], this is due to a marginally irrelevant operator in the field theory description, which causes strong finite-size effects. Increase the chain length to, e.g., $N = 120$ or 160. Do you observe the slow convergence behavior shown in Fig. 2(b) of Ref. [1]?

(d) To suppress finite-size effects at the Heisenberg point, consider the J_1-J_2 chain, where the marginal operator vanishes at $J_2/J_1 \simeq 0.24$. Compute the crosscap overlap for $N = 100$, $J_1 = 1$, and several values of $J_2 \in (0, 0.24)$. Compare your results with Fig. 3(c) in Ref. [1].

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