Theory

Infinite DMRG Algorithm

The Infinite Density Matrix Renormalization Group (DMRG) algorithm is a powerful method for obtaining ground state properties of one-dimensional quantum systems. The key idea is to iteratively build up the system size while keeping the most significant states that contribute to the ground state.

- **Initialization:** Start with a small system (usually two sites) and represent the system by its Hamiltonian.
- **Growth:** Increase the system size by adding two sites (one on each side) and form the superblock.
- **Truncation:** Diagonalize the Hamiltonian of the superblock and obtain the ground state wavefunction. Calculate the reduced density matrix of one half of the superblock and retain the most significant states to form a new truncated basis.
- **Iteration:** Repeat the growth and truncation steps until the desired system size is reached.

The infinite DMRG algorithm is particularly effective for systems with translational symmetry and provides a good starting point for the finite DMRG algorithm.

Finite DMRG Algorithm

- **Warmup Phase:** Run the infinite-size algorithm until the desired system size is reached. During this process, store all the left and right blocks, with their corresponding operators and basis transformations.
- **DMRG Sweeps:** Once the desired system size is reached, perform "DMRG sweeps", which involve iteratively optimizing the bases by sweeping from right-to-left and then from left-to-right across the system to improve accuracy.
- **Left-to-Right Sweep:** During a left-to-right sweep, the following steps are carried out:

1. **Add a site to the left block:** Add a site to the left block using the same idea as in the infinite-size DMRG. Since the total size of the system needs to be kept fixed, "shrink" the right block by using the smaller right block from the infinite-size step or from the previous right-to-left sweep.
2. **Diagonalize the super Hamiltonian:** Using a suitable library routine (Lanczos, Davidson), diagonalize the super Hamiltonian of the two blocks combined, similar to the infinite-size DMRG.
3. **Calculate the reduced density matrix:** Compute the reduced density matrix of the left block from the ground state wavefunction obtained by diagonalization.
4. **Diagonalize the density matrix:** Obtain the full spectrum and eigenvectors by diagonalizing the density matrix.
5. **Truncate the basis:** Retain only the m eigenvectors with the largest eigenvalues to form a new, truncated basis that captures the most significant degrees of freedom.
6. **Rotate the Hamiltonian and operators:** Rotate the Hamiltonian and the operators of the left block involved in interactions between blocks to the new basis.
7. **Iterate to the right end:** Continue the process iteratively until reaching the far right end of the system, where the right block contains a single site. This completes the left-to-right sweep.

- **Right-to-Left Sweep:** Perform a right-to-left sweep by growing the right block one site at a time, and using the left block from the previous left-to-right sweep. This involves similar steps to those in the left-to-right sweep but in the opposite direction.
- **Reiterate Sweeping:** Continue the sweeping process by alternating between left-to-right and right-to-left sweeps. Each sweep refines the approximation of the ground state. Stop when the change in the energy between sweeps falls below a predefined tolerance, indicating convergence. Typically, one stops when both blocks have the same size, known as the "symmetric configuration".
- **Advantages and Applications:** The finite DMRG algorithm is advantageous for its high accuracy in computing the ground state properties of one-dimensional quantum systems with short-range interactions. It is widely used in the study of spin chains, fermionic systems, and other condensed matter

systems. The finite DMRG is particularly effective in dealing with systems with open boundary conditions and can be adapted to study excited states and time-dependent phenomena.

- **Challenges and Limitations:** Despite its success, finite DMRG has limitations, particularly when dealing with two-dimensional systems or systems with long-range interactions. The computational cost increases with the size of the retained basis m, and for highly entangled systems, a large m is required, which can be computationally expensive. Extensions and modifications, such as the density matrix renormalization group with matrix product states (DMRG-MPS), have been developed to address some of these challenges.

Results

In the first problem, we solve the Ising Model with Hamiltonian:

$$H = -J \sum_i \sigma_i^z \sigma_{i+1}^z - h \sum_i \sigma_i^x \tag{1}$$

where:

- J is the coupling constant between neighboring spins.
- h is the transverse magnetic field.
- σ_i^z and σ_i^x are the Pauli matrices at site i.

In this Hamiltonian:

- The first term $-J \sum_i \sigma_i^z \sigma_{i+1}^z$ represents the interaction between neighboring spins in the z-direction.
- The second term $-h \sum_i \sigma_i^x$ represents the effect of the transverse magnetic field in the x-direction.

At the critical point $J = h$, the system undergoes a phase transition.

Ground State Energy

As we see, the value of ground state energy improves with each sweep:

Step	Value
Infinite DMRG	−29.4785169073468
Before Sweep	−29.417457469302583
Before Sweep	−29.417457470171406
Sweep 1	−29.351936371316445
Sweep 2	−29.325255451372605
Sweep 3	−29.312613382436535
Lanczos Method	−29.311821894762456

Correlation Functions

The correlation functions in the middle of every sweep are shown below:

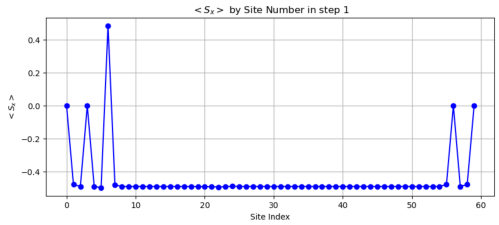

Figure 1: Sweep 1

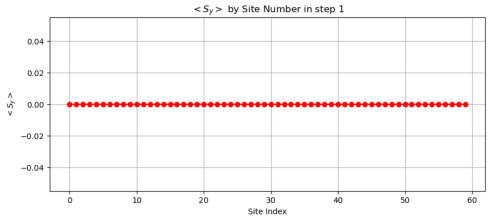

Figure 2: Sweep 2

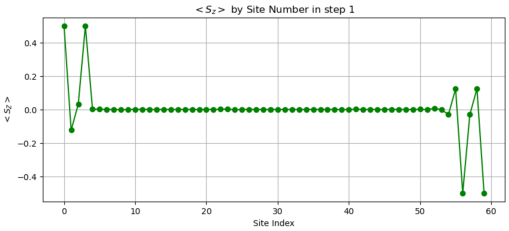

Figure 3: Sweep 3

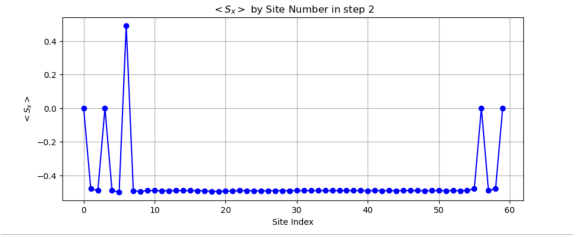

Figure 4: Sweep 4

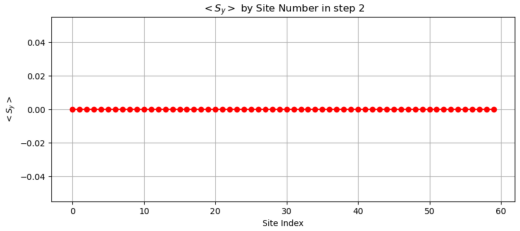

Figure 5: Sweep 5

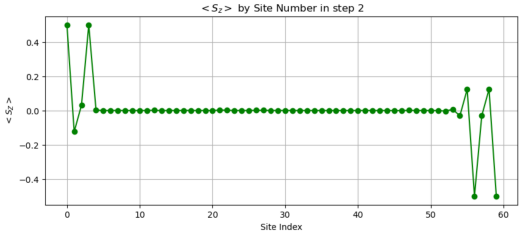

Figure 6: Sweep 6

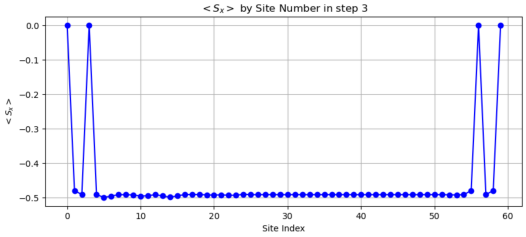

Figure 7: Sweep 7

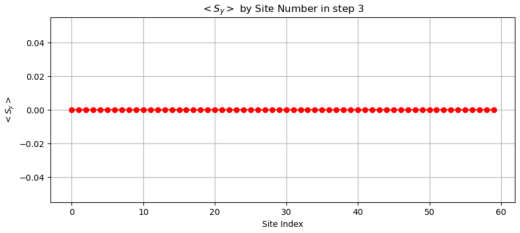

Figure 8: Sweep 8

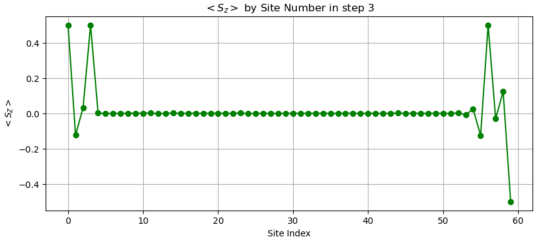

Figure 9: Sweep 9