DMRG study of Quantum Spin Systems

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1 Introduction

One of the most interesting research topics in many-body physics is the strongly correlated systems [1]. The simplest model of such systems is the single-band Hubbard model. Its Hamiltonian consists of the kinetic energy term and the on-site Coulomb repulsion term, which reads

$$\hat{H}_{\text{Hubbard}} = -\sum_{\langle ij\rangle,\sigma} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}. \tag{1}$$

The amplitude of electron hopping between site i and site j is t_{ij}, $\langle ij\rangle$ means site i and site j are nearest neighbours, and U denotes the on-site repulsion strength. In the limit $U/t \gg 1$, the double occupancy state $|\uparrow\downarrow\rangle$ should be excluded, which results in the $t-J$ model Hamiltonian

$$\hat{H}_{\text{tJ}} = -\sum_{\langle ij\rangle,\sigma} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}) + \sum_{\langle ij\rangle} J_{ij}(\mathbf{S}_i\cdot\mathbf{S}_j - \frac{1}{4}n_i n_j). \tag{2}$$

where $J_{ij} = 4{t_{ij}}^2/U$. And futhuremore, at half-filling, the $S = \frac{1}{2}$ Heisenberg Hamiltonian will be obtained

$$\hat{H}_{\text{Heisenberg}} = \sum_{\langle ij\rangle} J_{ij}\mathbf{S}_i\mathbf{S}_j. \tag{3}$$

The antiferromagnetic Heisenberg model is one of the most important quantum spin systems, which will be studied later using the density-matrix renormalization group (DMRG) method.

The most beautiful thing in theoretical condensed matter physics is that we can use a simple model Hamiltonian to capture many complex physical phenomena [2]. The spin systems can play such a role. As we've already known, Ising models have given us a full understanding of thermal phase transitions and critical phenomena. Currently, quantum spin systems like the antiferromagnetic Heisenberg model are forming a theoretical framework for exotic ground states and quantum phase transitions. Although simplified, quantum spin systems still well describe properties of some specific materials. The Heisenberg models have been very successful in explaining the antiferromagnetic properties of many Mott insulators. The most famous example is the undoped parent compounds of high T_c cuprates [3]. The quantum spin systems with frustrated or non-uniform interations can give us exotic ground states [4]. For example, the Heisenberg model in a triangle lattice gives us a disordered quantum spin liquid phase at zero temperature. The Heisenberg models are also closely related to quantum information theory [5]. For instance, the concept entanglement is widely used to describe

the properties of the antiferromagnetic Heisenberg model. In quantum spin systems, quantum phase transitions can also be observed, like in $J-Q$ models [6].

In classical statistical mechanics, Ising model and other classical models can be well simulated using Monte Carlo algorithm. However, when it comes to quantum many-body physics, people realize that it becomes much more difficult to find out a generic algorithm to simulate quantum spin systems. A few special one-dimensional models can be solved exactly. For most models, however, analytical solutions are based on approximations and assumptions. So it is necessary to use pure numerical simulation to verify the analytical solutions. The three core numerical algorithms for quantum spin systems are exact diagonalization (ED), quantum Monte Carlo (QMC) [7], and DMRG. I already have much experience in ED and QMC [8]. It's interesting that I study the antiferromagnetic Heisenberg chain using DMRG this time. It completes the numerical techniques I've mastered and I also can compare results from different algorithms. The model Hamiltonian can be represented by a matrix in some complete and orthogonal basis. If the eigenvalues and eigenvectors are obtained, all the information about the quantum system will be known. Unfortunately, because the size of the Hilbert space increases exponentially as the size of the system becomes larger, ED can only diagonalize a very small system. For some large-scale simulations, QMC can be applied. Because of the sign problem, QMC cannot be used to simulate quantum spin systems with frustrated interations. Finally, DMRG is a powerful and versatile computational tool but the drawback is that it just works out well for one-dimensional systems. Many physicists are taking efforts to figure out a DMRG scheme for two-dimensional systems.

The theory behind DMRG is mainly quantum information theory, e.g. density matrices and matrix product states. But I am not going deeply into it. The primary aim of this report is to introduce the DMRG algorithm, how to implement it and its application to the antiferromagnetic Heisenberg chain. Besides the static properties of one-dimensional systems at zero temperature, DMRG has many other applications. We also have dynamical DMRG, which can be used to investigate on the dynamical properties. Beyond real space lattices, we can use DMRG in the momentum space too. Transfer matrix DMRG can be applied to study systems at finite temperatures and time-dependent DMRG can work out for systems out of equilibrium. In addition, DMRG has othe applications, e.g. in quantum chemistry and nuclear physics.

2 Model

The Hamiltonian of the antiferromagnetic Heisenberg model shown in Eq. (3) can also written in another way

$$\hat{H}_{\text{Heisenberg}} = \sum_{\langle ij \rangle} J_{ij}[S_i^z S_j^z + \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+)] \tag{4}$$

As we can see, the Hamiltonian consists of two parts. The first part $S_i^z S_j^z$ support the maximally ordered antiferromagnetic state, i.e. $|\uparrow\downarrow\uparrow\downarrow ...\rangle$.The antiferromagnetic order will be reduced or totally destroyed by the second part $\frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+)$. It can be easily seen that the raising and lowering operators in the second part will cause local defects by flipping spin pairs. The amount of antiferromagnetic order remaining in the true ground state depends on the details of the lattice and interactions included in the Hamiltonian.

Now just consider the antiferromagnetic Heisenberg interation between site i and site j ($N = 2$)

$$\hat{H}_{ij} = J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j \tag{5}$$

The maximally ordered antiferromagnetic state $|\uparrow\downarrow\rangle$ is the eigenstate with an eigenvalue $-\frac{1}{4}J_{ij}$, while the singlet state $\frac{|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle}{\sqrt{2}}$ is the eigenstate with an eigenvalue $-\frac{3}{4}J_{ij}$. It means that the antiferromagnetic Heisenberg interation tends to support the singlet state. When $N > 2$, there doesn't exist a ground state where all the nearest neighbours form singlet pairs. However, it has been verified that the ground state is a superposition of all the states which are product states of $\frac{N}{2}$ singlet states [**?**]. This superposition state is called valence-bond state.

3 Numerical Method

The basic idea of the DMRG algorithm is a truncation scheme without losing information about the quantum systems, as shown in Figure.1. For the system of length l, we have an M^S-dimensional Hilbert space with states $\{|m_l{}^s\rangle\}$. A matrix is used to represent the Hamiltonian and its elements should be $\langle m_l{}^s|\hat{H}_l|\tilde{m_l}{}^s\rangle$. Similarily, we can also build matrices representing local operators the same way. Then one new site is added to the system. Then in the new product basis ($\{|m_l{}^s\sigma\rangle\} \equiv \{|m_l{}^s\rangle|\sigma^s\rangle\}$), the new Hamlitonian $\hat{H}_{l+1}$ and other local operators are built. The same thing should be done for the environment, after which a superblock of length $2l+2$ is obtained. After diagonalizing the Hamiltonian matrix for the superblock, the ground state is calculated

$$|\psi\rangle = \sum_{m^S=1}^{M^S}\sum_{\sigma^S=1}^{N_{\text{site}}}\sum_{\sigma^E=1}^{N_{\text{site}}}\sum_{m^E=1}^{M^E}\psi_{m^S\sigma^S\sigma^E m^E}|m^S\sigma^S\rangle|m^E\sigma^E\rangle \equiv \sum_{i}^{N^S}\sum_{j}^{N^E}\psi_{ij}|i\rangle|j\rangle \tag{6}$$

Reduced density matrix is used to describe physical properties of the system

$$\hat{\rho} = \text{Tr}_E|\psi\rangle\langle\psi| \tag{7}$$

Its elements can be calculated in the following way

$$\langle i|\hat{\rho}|i'\rangle = \sum_j \psi_{ij}\psi^*_{i'j} \tag{8}$$

Futuremore, we diagonalize the reduced density matrix for the system $\hat{\rho}|w_\alpha\rangle = w_\alpha|w_\alpha\rangle$, with $\sum_\alpha w_\alpha = 1$ and $w_\alpha \geq 0$. Then we can sort them as $w_1 \geq w_2 \geq w_3 \geq \ldots$.The physical meaning of the eigenvalues w_α is that w_α of the state is $|w_\alpha\rangle$. When we calculate the expectation value for some operator, we can just take into account the first several states and ignore the rest. We can also truncate the Hamiltonian and other local operators this way, which will be illustrated later.

As shown in Figure.1, we can keep adding sites to the system and keep the size of the Hilbert space invariant, until the size of the superblock reaches the size of the system. It's called infinite-system DMRG. If we just study the static properties of the ground state, the implementation procedure is as follows [1]

1. Consider a lattice of some small size l, forming the system block S. S lives on a Hilbert space of size M^S with states $\{|m_l^s\rangle\}$; the matrices representing the Hamiltonian $\hat{H}_l$ and the operators acting on the block can be calculated in this basis. Similarly, form an environment block E.

2. Form a tentative new system block S′ from S and one added site. S′ lives on a Hilbert space of size$N^S = M^S N_{\text{site}}$, with a basis of product states $\{|m_l^s\sigma\rangle\} \equiv \{|m_l^s\rangle|\sigma\rangle\}$. In principle, the Hamiltonian $\hat{H}_{l+1}$ acting on S′ can now be expressed in this basis. A new environment E′ is built from E in the same way.

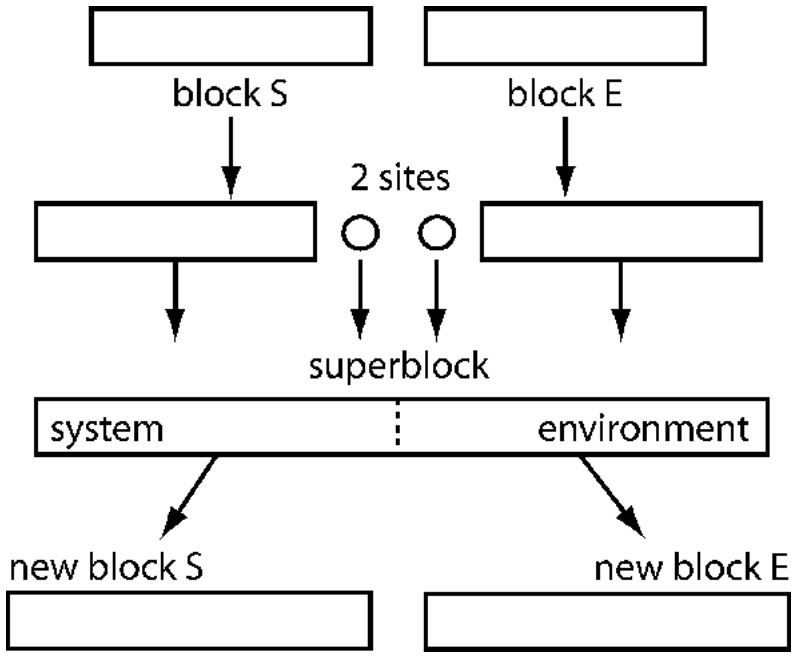

Figure 1: The system meets the environment and both of them form a superblock together. After the truncation, new blocks are formed, which keep the same size of Hilbert space and include one more site.

3. Build the superblock of length $2l+2$ from S′ and E′. The Hilbert space is of size $N^S N^E$, and the matrix elements of the Hamiltonian $\hat{H}_{2l+2}$ could in principle be constructed explicitly.

4. Find by exact diagonalization of $\hat{H}_{2l+2}$ the ground state $|\psi\rangle$. This is the most time-consuming part of the algorithm.

5. Form the reduced density-matrix $\hat{\rho} = \mathrm{Tr}_E|\psi\rangle\langle\psi|$ as in Eq. (7) and determine its eigenbasis $|w_\alpha\rangle$ ordered by descending eigenvalues (weight) w_α. Form a new (reduced) basis for S′ by taking the M^S eigenstates with the largest weights. In the product basis of S′, their matrix elements are $\langle m_l^s \sigma | m_{l+1}^s \rangle$; taken as column vectors, they form a $N^S \times M^S$ rectangular matrix T. Proceed likewise for the environment.

6. Carry out the reduced basis transformation $\hat{H}_{l+1}^{\mathrm{tr}} = T^\dagger \hat{H}_{l+1} T$ onto the new M^S-state basis and take $\hat{H}_{l+1}^{\mathrm{tr}} \to \hat{H}_{l+1}$ for the system. Do the same for the environment and restart with step (2) with block size $l+1$ until some desired final length is reached. Operator representations also have to be updated.

7. Calculate desired ground state properties (energies and correlations) from $|\psi\rangle$; this step can also be carried out at each intermediate length.

However, for most problems, the infinite-system DMRG cannot give satiesfactory results. To improve this, the finite-system DMRG should be conducted after the infinite-system DMRG.In the infinite-system DMRG part, we add two more sites to the superblock each time until the size of the superblock reaches its limit, the size of the quantum many-body system. However, in the finite-system DMRG part, we have to keep the size of the superblock, which means if we include one more site

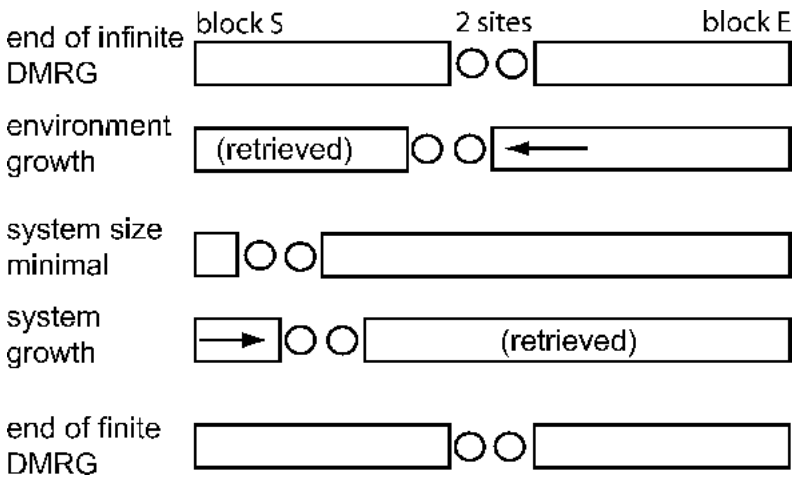

Figure 2: It illustrates the procedure of the finite-system DMRG.

to the system we should take away one site from the environment. As illustrated in Figure.2, we keep adding sites to the system while taking away sites from the environment until the size of the environment arrives at its minimum limitation (when the minimum limitation is reached, we say one halfsweep has been finished). Then we exchange the roles of the system and the environment. We keep doing this till the results converge to the precision we want.

After the infinite-system DMRG is finished (in the part, we should store the matrix representing the block Hamiltonian of length l as B_l), the implementation procedure for the finite-system DMRG is listed in the following [9]

1. Set $l = L/2$. Use B_l as block S and the reflection of B_{L-l-2} as block E.
2. Steps 2-6 as in the infinite-system DMRG part.
3. Store the new block S as B_{l+1}, replacing the old B_{l+1}.
4. If $L - l - 2 > m$ (m is the minimum limitation of the size of the environment), set $l = l + 1$ and go to step 2.
5. If $L-l-2 = m$, exchange the roles between the system and the environment and one halfsweep is finished. Keep sweeping into the opposite direction.

4 Implementation

I applied DMRG to study the antiferromagnetic Heisenberg chain with open boundary conditions. Before I write the main function, I make several important sub-functions in four header files. Firstly, in *tensor.hpp*, the function *MatrixXd tensor_ product(MatrixXd A, MatrixXd B)* calculate the tensor product between the matrix A and the matrix B. Before it, there is a function *int power(int x, int y)* which calculate x^y. Secondly, in *ED.hpp*, the function *int index_ min(VectorXd A)* returns the index of the minimum value among an array of numbers. The function *VectorXi sort_ vector(VectorXd A)* sort an array of numbers and then return the indices. The function *double groundstate(MatrixXd H,*

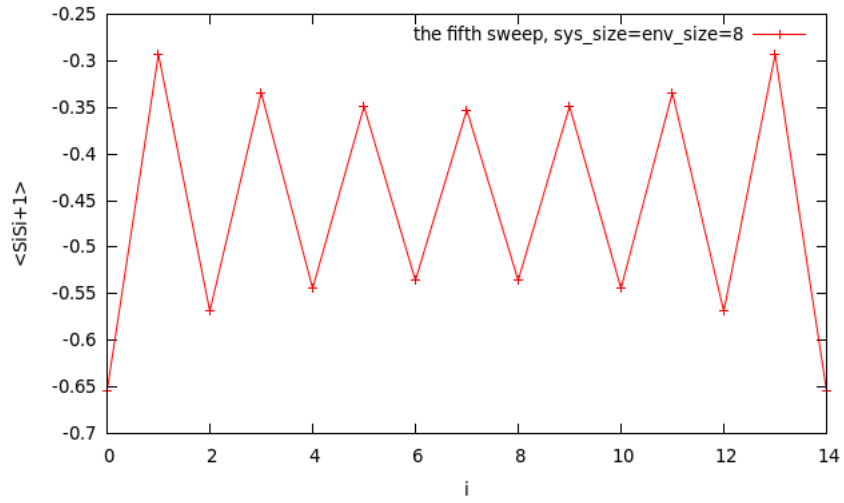

Figure 3: Local bond strengths, L=16.

VectorXd& evec) diagonalize the matrix H, obtaining the ground state and its corresponding energy. The last function *void diagonalization(MatrixXd D, VectorXd& eval, MatrixXd& evec)* will get all the sorted eigenstates and their corresponding eigenvalues of the matrix D. Thirdly, in *RDM.hpp*, the function *MatrixXd reduced_ density_ matrix(VectorXd evec, int n)* calculates the reduced density matrix for the system from the ground state. The vector evec is 2^{2n}-dimensional and the returned reduced density matrix should be $2^n \times 2^n$. The function *MatrixXd transformation_ matrix(MatrixXd density, int m)* will calculate the transformation matrix T from the reduced density matrix. Finally, in *WR.hpp*, the first function *void save(const char *filename, const MatrixXd& m)* will save a matrix m into a binary file and the second function *void load(const char *filename, MatrixXd& m)* will load from a binary file and save the matrix in m. The function *void infinite_ write(vector<MatrixXd> correlation, int system_ size)* will save an array of matrices representing the nearest-bonds into some binary files during the infinite-system DMRG part, while the function *void finite_ write(vector<MatrixXd> correlation, int system_ size, int iter)* will do the same thing during the finite-system DMRG part. During the finite-system DMRG part, the function *void finite_ read(vector<MatrixXd>& correlation, int system_ size, int iter)* then read the array of matrices representing the nearest-bonds from the binary files we wrote previously. The final function *void printf_ bonds(vector<MatrixXd> nearest_ correlation, VectorXd evec, int iter, int system_ size)* will write the nearest neighbour spin-spin correlations into a *.txt* file. I also write the program *test.cpp* to make sure all the sub-functions work out perfectly right. The main function is in *heisenberg.cpp*. After compiling it, we should run the program as $.\backslash heisenberg$ *16 4 5*, where the size of the chain is 16, 2^4 states will be kept after each trunction and 5 halfsweeps should be finished. By running the program, we can obtain the ground state energy and nearest neighbour correlations.

5 Benchmark Calculations

By running $.\backslash heisenberg$ *16 4 5*, we obtain the converged ground state energy is $E_0/L = -0.4319835$, which is very close to the exact result from Bethe Ansatz $E_0/L = -0.4319357$. And we also calculate the bond strengths in the chain, as shown in Figure.3.

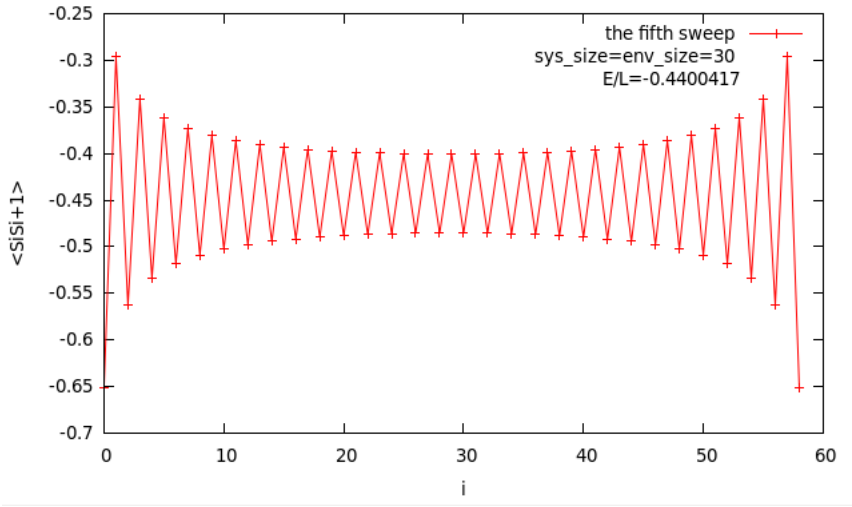

Figure 4: Local bond strengths, L=16.

6 Results

I also run .\$heisenberg$ *60 4 5*, which takes around 10 hours. The results are shown in Figure.4.

7 Discussion

We compare the ground state energy for L=16 with that from the exact solution and verify the validity of my DMRG codes. From Figure.3 and Figure.4, we realize that the local bonds have different strengths, which we believe comes from the finite-size effect and the open boundary condition. It's expected that local bonds should share the same strength for the chain with periodic boundary conditions. In addition, in the chain with periodic boundary conditions, we can mearsure the long-range spin-spin correlations. Another thing we can do is to calculate the ground state energy for different L's and anylize the result when L goes to infinite. It's worth mentioning that my program runs slow, which I think is from writing to and reading from the disk.

References

[1] U. Schollwock, Rev. Mod. Phys. **77**, 259 (2005).

[2] A. W. Sandvik, AIP Conf. Proc. **1297**, 135 (2009).

[3] E. Manousakis, Rev. Mod. Phys. **63**, 1 (1991).

[4] L. Balents, Nature **464**, 199 (2010).

[5] M. B. Hastings, I. Gonzalez, A. B. Kallin, and R. G. Melko, Phys. Rev. Lett. **104**, 157201 (2010).

[6] A. W. Sandvik, Phys. Rev. Lett. **104**, 177201 (2010).

[7] A. W. Sandvik, Phys. Rev. Lett. **95**, 207203 (2005).

[8] J. Xu, Monte Carlo Study of Quantum Spin Systems, Bachelor's Thesis.

[9] S. R. White, Phys. Rev. B, **48**, 10345 (1993).