Università degli Studi di Padova - January 8, 2024
Dipartimento di Fisica e Astronomia "G. Galilei"
Quantum information and computing

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Assignment 8

Introduction

The Real Space Renormalization Group (RSRG) and the Density Matrix Renormalization Group (DMRG) are powerful techniques in theoretical physics and quantum mechanics used to study complex systems. Both methods offer crucial insights into diverse fields, from condensed matter physics to quantum chemistry, enabling a deeper understanding of the behavior of matter at different scales.

1 Real Space Renormalization Group

Real-space renormalization group method is an approximation method based on a very powerful physical intuition: the hypothesis that the ground state of a system is composed of low-energy states of the system's (non-interacting) bipartitions. Based on this assumption, it is indeed possible to introduce an algorithm that allows describing the ground state properties of many-body quantum systems with large sizes N.

The algorithm proceeds as follows:

1. Begin by considering a system composed of N sites that can be studied numerically with exactness. Create the Hamiltonian $\mathcal{H}_N$ for this system.

2. Proceed to diagonalize $\mathcal{H}_N$ to find its eigenvalues and eigenvectors, represented by $\mathcal{H}_N = \sum_{i=1}^{d^N} E_i |v_i\rangle\langle v_i|$, where the eigenvalues E_i are arranged in ascending order. Form a projector P onto the lowest d^N eigenstates, $P = \sum_{i=1}^{d^N} |v_i\rangle\langle v_i|$, which projects the Hilbert space onto the subspace defined by these low-energy states. Calculate the projected Hamiltonian $\mathcal{H}_N^{pr} = P^\dagger \mathcal{H}_N P$ and any other required operator representation within this projected space, denoted as $\mathcal{O}^{pr} = P^\dagger \mathcal{O} P$.

3. Construct the Hamiltonian for a system of size $2N$ utilizing the projected Hamiltonian $\mathcal{H}^{pr}$ for each bipartition and the interactions between them. Express this as $\mathcal{H}_{2N} = \mathcal{H}_N^{pr} \otimes \mathbb{I}_N + \mathbb{I}_N \otimes \mathcal{H}_N^{pr} + A_N \otimes B_N$. Obtain the interaction Hamiltonian $\mathcal{H}_{int} = A^{pr} \otimes B^{pr}$ where A^{pr} and B^{pr} represent the projected operators acting on each system bipartition, derived from $A^{pr} = P^\dagger A P$ and $B^{pr} = P^\dagger B P$.

4. Iterate through steps 1–3 until reaching the desired system size or achieving convergence to the renormalization group's fixed point. Note that in each iteration, the system's size doubles ($N \to 2N$), while the Hamiltonian representation remains constant at d^N.

1.1 Implementation

The goal is to apply the theory (sec. 1) to the 1-D spin-$\frac{1}{2}$ chain described by the following Hamiltonian (eq. 1).

$$H = \lambda \sum_i \sigma_z^i + \sum_i \sigma_x^i \sigma_x^{i+1}. \tag{1}$$

We start from n=0 (zero iteration):

$$H_N^{(0)} = \lambda \sum_i \sigma_z^i + \sum_i \sigma_x^i \sigma_x^{i+1}, \tag{2}$$

$$A^{(0)} = \mathbb{I}_{N-1} \otimes \sigma_x, \tag{3}$$

$$B^{(0)} = \sigma_x \otimes \mathbb{I}_{N-1}. \tag{4}$$

At this point, we consider an exact copy (B) of the system A. Look figure 1.

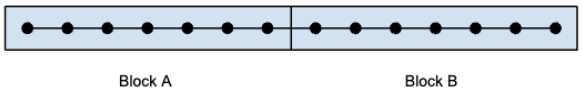

Figure 1: Two identical blocks of spin A and B connected with and interaction of the kind $\sigma_x \otimes \sigma_x$.

From the previous step, it is possible to build the Hamiltonian for the system of size 2N (5).

$$H_{2N}^{(n)} = H_N^{(n)} \otimes \mathbb{I}_N + \mathbb{I}_N \otimes H_N^{(n)} + A_N^{(n)} \otimes B_N^{(n)}. \tag{5}$$

We proceed with the calculation of the projector as shown in the follow (6):

$$P = \sum_{i=1}^{d^N} |v_i\rangle\langle v_i|. \tag{6}$$

We compute the energy density: $\epsilon = E_o/N$, where N is considered as the number of particles at the n-th iteration. Compare this value against a threshold, τ, to check if the convergence criteria are met (eq. 7).

$$\Delta n = |\epsilon(n) - \epsilon(n-1)| < \tau \tag{7}$$

If it is not converged: update the Hamiltonian and the interaction for the next iteration.

$$H_N^{n+1} \leftarrow \frac{1}{2} P^\dagger H_{2N}^n \frac{1}{2} P \tag{8}$$

$$A_N^{n+1} \leftarrow \frac{1}{\sqrt{2}} P^\dagger (\mathbb{I}_N \otimes A_n^N) P \tag{9}$$

$$B_N^{n+1} \leftarrow \frac{1}{\sqrt{2}} P^\dagger (B_N^n \otimes \mathbb{I}_N) P \tag{10}$$

1.2 Results

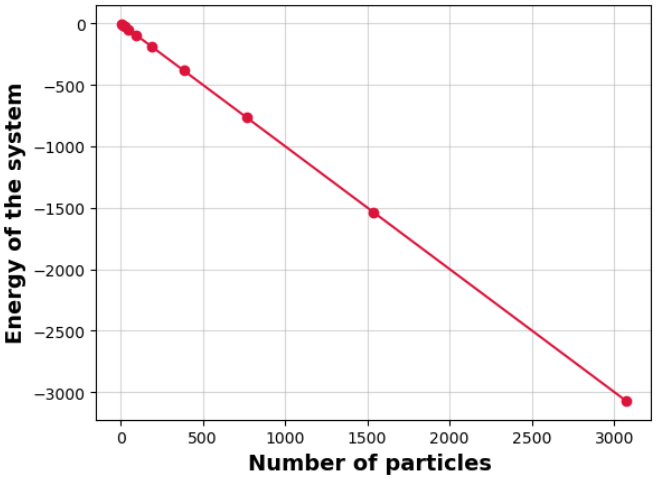

Figure 2: Energy of the system as a function of the number of particles.

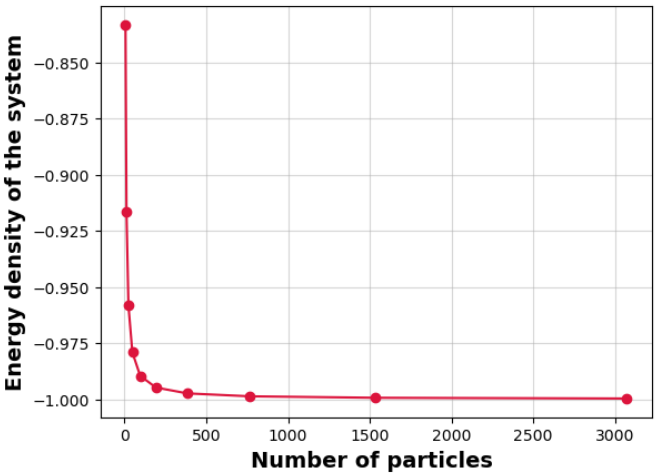

Figure 3: Energy density of the system as a function of the number of particles.

The graph 2 accurately represents the system's behavior by showcasing that when the system doubles in size, its energy also doubles. Graph 3 shows the energy density of the system reaching the asymptotic behavior -1.

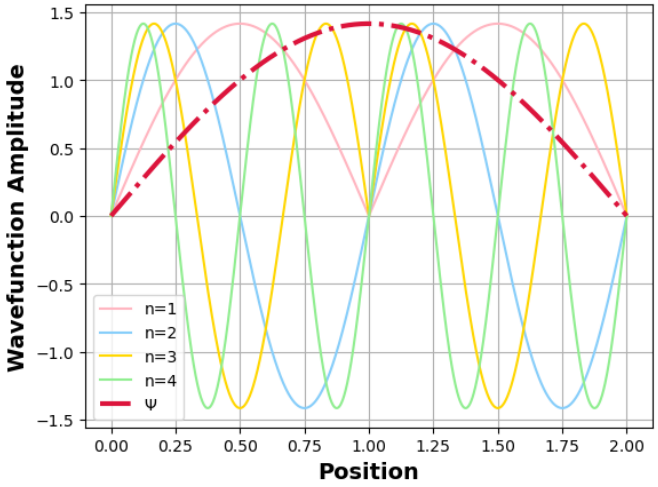

Figure 4: Solution of the problem describing a particle in infinite box potential. The graph reports the solutions of the single-half ($x \in [0, 1]$) system and also the first eigenstate of the doubled system ($\Psi(x)$) with $x \in [0, 2]$.)

The Real Space Renormalization Group (RSRG) encounters limitations in certain scenarios, such as the example of a particle in a box (fig. 4), where reproducing the full wavefunction $\Psi(x)$ becomes impossible using only a finite number of eigenstates from one half of the system.

2 Density Matrix Renormalization Group

The DMRG is a powerful modification of the original RG algorithm, where the truncation rule is improved resulting in a higher precision description of the final state at the price of slowing down the growth of the system size. Indeed, in the DMRG algorithm, the system size increases linearly instead of exponentially with the number of iterations. We consider the system described by equation 1. The algorithm, developed to describe such a problem is composed of the following steps: We start considering a global system composed of 4 parts: Left (L) and right (R) blocks containing $m + 1$ sites each (fig. 5).

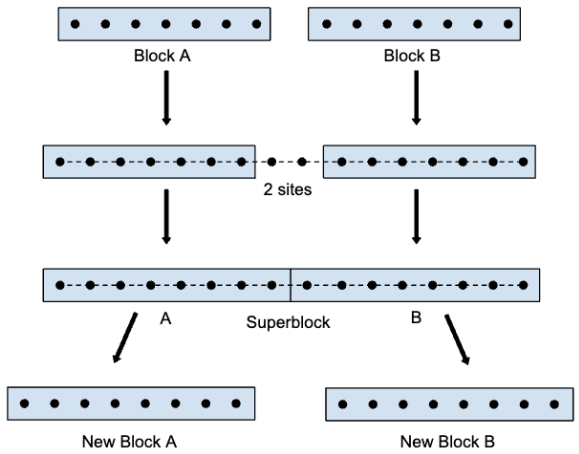

Figure 5: A sketch of step 1-st of the Infinite DMRG algorithm.

We initialize some operators as follows:

$$\mathcal{H}_L^{(0)} = \lambda\sigma_z, \tag{11}$$
$$\mathcal{H}_R^{(0)} = \lambda\sigma_z, \tag{12}$$
$$A_L^{(0)} = \mathbb{I}_1, \tag{13}$$
$$B_L^{(0)} = \sigma_x, \tag{14}$$
$$\mathcal{H}_2^{(0)} = \lambda\sigma_z, \tag{15}$$
$$\mathcal{H}_3^{(0)} = \lambda\sigma_z. \tag{16}$$

We enlarge the left (right) block by adding one site:

$$\mathcal{H}_{L+1}^{(n)} = \mathcal{H}_L^{(n)} \otimes \mathbb{I}_1 + A_L^{(n)} \otimes \mathcal{H}_2 + B_L^{(n)} \otimes \sigma_x^i, \tag{17}$$
$$\mathcal{H}_{R+1}^{(n)} = \mathbb{I}_1 \otimes \mathcal{H}_R^{(n)} + \mathcal{H}_3 \otimes A_R^{(n)} + \sigma_x^i \otimes B_R^{(n)}. \tag{18}$$

We update:

$$A_{L+1}^{(n)} = \mathbb{I}_m, \tag{19}$$
$$B_{L+1}^{(n)} = \mathbb{I}_{m-1} \otimes \sigma_x. \tag{20}$$

We build the Hamiltonian for 2m + 2 particles:

$$\mathcal{H}_{2m+2}^{(n)} = \mathcal{H}_{L+1}^{(n)} \otimes \mathbb{I}_{R+1} + \mathbb{I}_{L+1} \otimes \mathcal{H}_{R+1}^{(n)} + \mathcal{H}_{L,R}^{(n)}. \tag{21}$$

where $\mathcal{H}_{L,R}^{(n)} = \mathbb{I}_m \otimes \sigma_x \otimes \sigma_x \otimes \mathbb{I}_m$. We diagonalize the full Hamiltonian and we construct the den-

sity matrix for the ground state $\rho = |GS\rangle\langle GS|$. After that, we compute the reduced density matrix for the left side of the system ρ_{L+1}. After, we diagonalize the ρ_{L+1} and using the first $l = min(2^m, 2^{m_{max}})$ eigenstates we build the projector P and $P^\dagger$. In the last step of the algorithm, we use P and $P^\dagger$ to project the left (right) operators needed for the next iteration.

$$\mathcal{H}_L^{n+1} \leftarrow P^\dagger \mathcal{H}_L^n P, \tag{22}$$

$$A_L^{n+1} \leftarrow P^\dagger A_n^L P, \tag{23}$$

$$B_L^{n+1} \leftarrow P^\dagger B_n^L P. \tag{24}$$

What remains to do is to iterate the procedure many times to enlarge the system up to the desired size. The energy is computed as shown in eq. 25

$$\epsilon = \frac{E_0}{2(m+1)}. \tag{25}$$

2.1 Results

In this section, the results obtained with the DMRG method are reported.

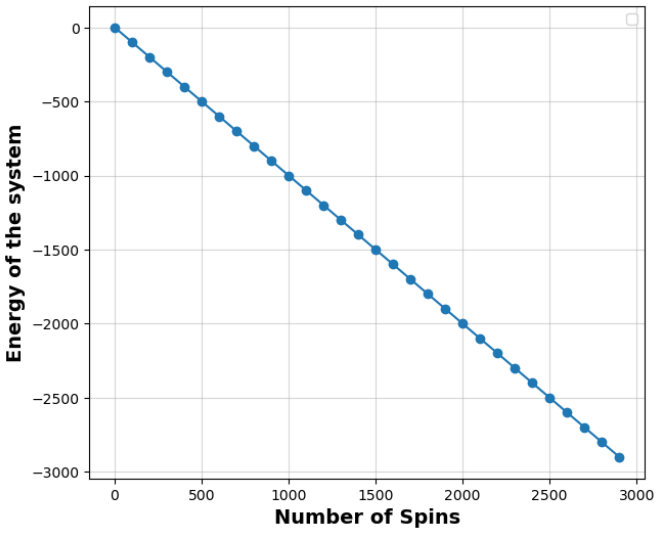

Figure 6: Energy of the system as a function of the number of particles.

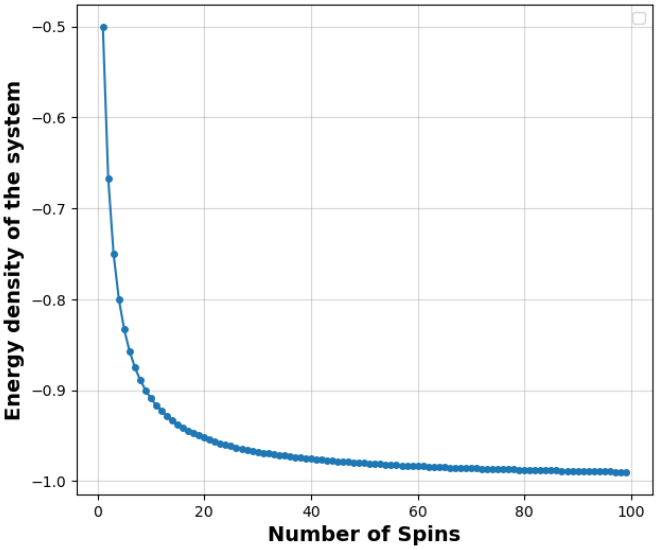

Figure 7: Energy density of the system as a function of the number of particles.

The considerations are analogous to the ones done in the RSRG case. The only difference is that the system size and also the energy scale linearly rather than exponentially.

Comparison and Conclusion

In this section, we will compare the results obtained with the RSRG and DMRG with the Mean Field version.

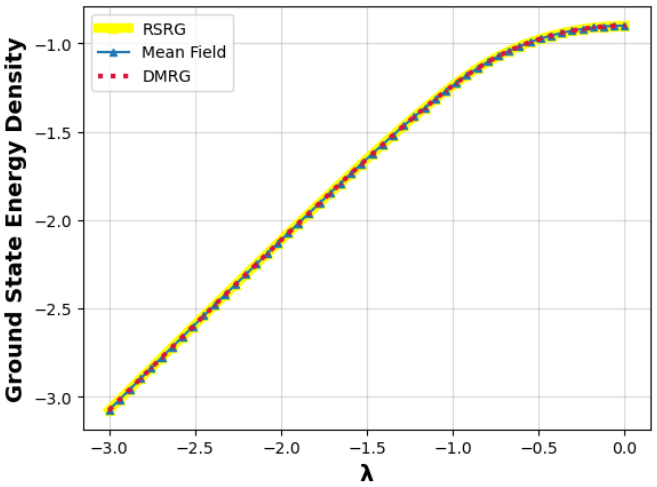

Figure 8: Overlap of the three curves obtained with RSRG, DMRG and Mean Field method. Each curve represents the ground state, of a 10-spin chain, as a function of the field λ.

In figure 8, we immediately see the "perfect" overlap of the three curves, namely the methods pro-

duce the same result in this particular case.

In summary, for a 10-spin system, Mean-Field (MF), Real Space Renormalization Group (RSRG), and Density Matrix Renormalization Group (DMRG) yield identical results. However, the advantages lie in scalability and computational efficiency. RSRG and DMRG facilitate the study of larger systems as the Hilbert space dimension remains fixed, resulting in computation time growing linearly with the number of particles. Conversely, MF suffers from exponential time scaling as the system size increases. In addition, the DMRG overcomes some limitations of the RSRG in dealing with system entanglement.