QUANTUM INFORMATION AND COMPUTING

Assignment 8

Author
Marco Chiloiro
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1 Real Space Renormalization Group

The Renormalization Group (RG) is a powerful theoretical framework applied to many-body systems. In this report, we study the application of Real Space Renormalization Group (RSRG) method, specifically in the context of a one dimensional transverse-field quantum Ising model.

1.1 Theoretical background

The Real Space Renormalization Group (RSRG) is based on the assumption that the ground state of a many-body system is composed of low-energy states of the bipartitions of the system. The idea behind the algorithm involves a truncation procedure based on energy considerations.

Consider a system composed of $2N$ bodies that can be numerically studied exactly. Now, construct the Hamiltonian acting on this system as follows:

$$\hat{H}_{2N} = \hat{H}_N^L \otimes \mathbb{1}_N + \mathbb{1}_N \otimes \hat{H}_N^R + \hat{H}^{\text{int}}, \tag{1}$$

where $\hat{H}_N^L$ is the Hamiltonian acting on the left subsystem of N bodies, $\hat{H}_N^R$ is the one acting on the right subsystem, and $\hat{H}^{\text{int}}$ represents the interaction between these two subsystems. If the Hilbert space for a single constituent body has dimension d (assumed identical for all), then $\hat{H}_{2N}$ will be a matrix of size $m^2 \times m^2$, where $m = d^N$.
Next, diagonalize $\hat{H}_{2N}$ and construct a projector $\hat{P}$ whose columns are formed by the m eigenvectors corresponding to the lowest m eigenvalues. Now, let us project $\hat{H}_{2N}$ using this projector,

$$\hat{H}_{2N}^{\text{trunc}} = \hat{P}^\dagger \hat{H}_{2N} \hat{P}, \tag{2}$$

resulting in a truncated Hamiltonian of size $m \times m$ describing the system composed by $2N$ bodies. By setting $\hat{H}_N^L = \hat{H}_{2N}^{\text{trunc}}$, it is possible to iterate this process until a convergence condition is reached. It is noteworthy that at each iteration step, a Hamiltonian representing a system of double the size of the previous step is obtained.
This method is effective if the underlying assumption holds true, namely, if the ground state is indeed composed of a superposition of low-energy states. While this assumption may not always be accurate, the method remains effective in many situations.
This methodology has been applied to the Hamiltonian

$$\hat{H} = \sum_{i=1}^{N-1} \sigma_i^x \sigma_{i+1}^x + h \sum_{i=1}^{N} \sigma_i^z, \tag{3}$$

where spin interactions along the x-axis occur only between nearest neighbors, and a magnetic field of magnitude h is applied along the z-axis.

1.2 Implementation

The *RealSpaceRG* function implements the Real-Space Renormalization Group (RSRG) transformation for a 1-dimensional transverse-field Ising model.
The function takes several parameters as input, such as the initial number of spins (N_0), the

maximum number of iterations (*num_iter*), a tolerance for convergence (*tol*), and a Hamiltonian function (H) that characterizes the quantum system. Additional parameters for the Hamiltonian can be provided through ***kwargs*. Built-in functions used include *isinstance()* for type checking, *np.eye()* for generating an identity matrix, *np.kron()* for computing tensor products, and *np.linalg.eigh()* for diagonalizing the Hamiltonian. Convergence is checked by comparing the ground energy per spin between iterations. If the difference falls below the specified tolerance, the algorithm stops. The function returns two arrays, e and N. The array e contains the ground energy per spin for each iteration, and the array N represents the number of spins for each iteration. Additionally, there is a commented warning that can be activated if the algorithm does not converge within the specified number of iterations.

1.3 Results

Consider the Hamiltonian given by (3). The magnetic field magnitudes h explored lie within the interval $h \in [-3, 0]$. Employing a tolerance of $\delta = 10^{-8}$, the algorithm converges after 26 iterations for all values of h in the specified interval. Figure 1 depicts the results post-convergence.

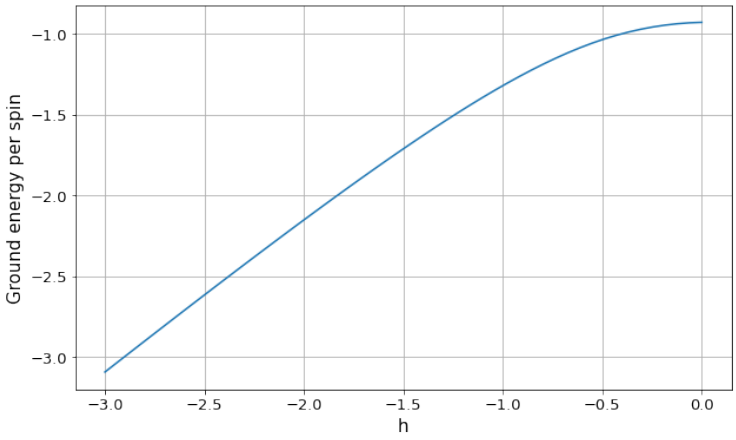

Figure 1: Ground state energy (E_0) per spin (E_0/N) as a function of the magnetic field intensity h. The initial system size is $N_0 = 2$. The algorithm achieves convergence after 26 iterations ($\delta = 10^{-8}$), resulting in a final system size of $N = 2^{27}$.

The shape of the curve aligns with our expectations, displaying an energy per spin around -1 for magnetic field values close to 0. Beyond the phase transition from antiferromagnetic to paramagnetic, which occurs around $h = -1$, the curve follows a linear trend.

Let us take a look at the convergence behavior. Figure 2 reveals that, for small magnetic field intensities, the algorithm begins at a more substantial distance from the convergence value compared to higher h values. Interestingly, for larger h, the ground state energy per spin stabilizes more rapidly, with minimal variation observed even in the early iteration steps.

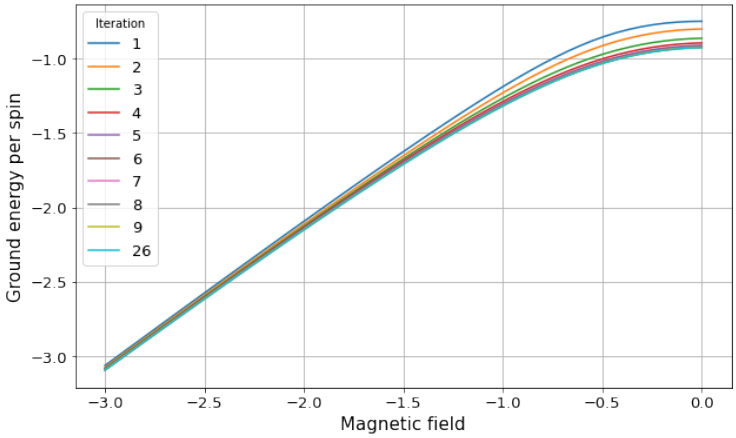

Figure 2: Ground state energy (E_0) per spin (E_0/N) as a function of the magnetic field intensity h for distinct iteration steps. The initial system size is $N_0 = 2$.

To further highlight this behavior, Figures 3 and 4 present a comparison, along with the relative absolute error, between the exact solution spins and the algorithm results for the same number of spins $N = 16$. In the first case, obtained with an initial system size of $N_0 = 2$, three iterations are needed to reach $N = 16$. Conversely, in the second case with $N_0 = 4$, two iterations suffice.

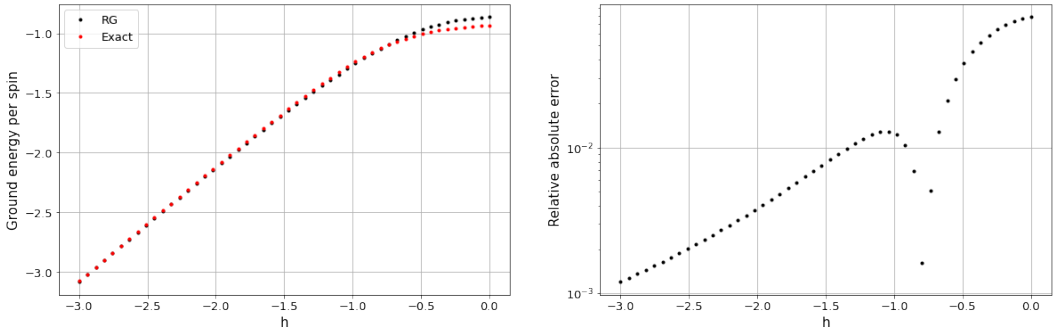

Figure 3: Comparison between exact and RSRG method after 3 steps solutions. Ground state energy per spin as a function of the magnetic field intensity h on the left, relative absolute error on the right. The initial system size is $N_0 = 2$.

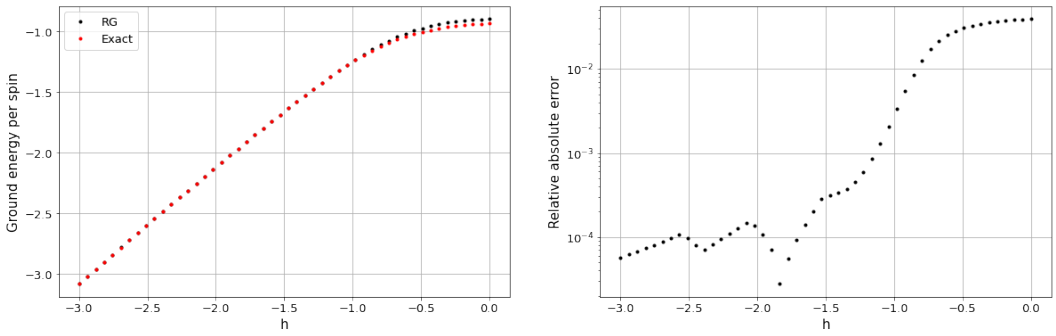

Figure 4: Comparison between exact and RSRG method after 2 steps solutions. Ground state energy per spin as a function of the magnetic field intensity h on the left, relative absolute error on the right. The initial system size is $N_0 = 4$.

The comparison reveals that the error is more pronounced for $N_0 = 2$, particularly for h values within the antiferromagnetic phase ($h > -1$). This discrepancy arises because, with $N_0 = 4$, we keep 2^4 eigenvectors instead of 2^2. The improvement in results with $N_0 = 4$ suggests that, with $N_0 = 2$, we overlook higher-energy terms that significantly contribute to the ground state, especially in the antiferromagnetic phase.

2 Density Matrix Renormalization Group

The Density Matrix Renormalization Group (DMRG) represents an enhancement of the Real Space Renormalization Group (RSRG) algorithm. This modification involves refining the truncation rule, leading to a more accurate representation of the final state. However, this increased precision comes at the cost of a reduced rate of system size expansion, resulting in a slower overall computation.

2.1 Theoretical Background

The following algorithm, named infinite DMRG, was developed to describe systems with nearest neighbors interactions at the thermodynamic limit.

Consider a system composed by a one-dimensional lattice of size N which can be solved exactly. Now, introduce an additional site to this system. Let us assume that each site has a physical dimension d. Then, the dimension of the Hilbert space of the system equals dm, where $m = d^N$. Double the system and construct the corresponding Hamiltonian $\hat{H}_{2N+2}$ of the form

$$\hat{H}_{2N+2} = \hat{H}^L_{N+1} \otimes \mathbb{1}_{N+1} + \mathbb{1}_{N+1} \otimes \hat{H}^R_{N+1} + \hat{H}^{\text{int}}, \tag{4}$$

where $\hat{H}^L_{N+1}$ is the Hamiltonian acting on the left subsystem of size $N+1$, $\hat{H}^R_{N+1}$ is the one acting on the right subsystem, and $\hat{H}^{\text{int}}$ represents the interaction between these two subsystems. The next step is to diagonalize $\hat{H}_{2N+1}$, finding the ground state of the system $|\psi_{\text{GS}}\rangle$. From this state, construct the corresponding density matrix

$$\rho = |\psi_{\text{GS}}\rangle\langle\psi_{\text{GS}}|. \tag{5}$$

From (5) compute the reduced density matrix of the left subsystem of size $N+1$:

$$\rho_L = \mathrm{Tr}_R \rho. \tag{6}$$

Now, diagonalize the reduced density matrix (6); the eigenvalues λ_i corresponds to the populations of the corresponding eigenstates $|w_i\rangle$. Select the m eigenstates corresponding to the m largest eigenvalues and use them to construct the projector $\hat{P}$. Finally, project the left Hamiltonian (7) and all necessary operators in the reduced space,

$$\hat{H}_{N+1}^{\mathrm{trunc}} = \hat{P}^\dagger \hat{H}_{N+1}^{L} \hat{P}. \tag{7}$$

We thus obtain an effective Hamiltonian describing the system of $N+1$ sites of dimension m instead of md. Iterate the process by replacing the left and right Hamiltonian terms with the new projected terms.
With each iteration, the size of the described system increases by two sites.

2.2 Implementation

The *QIM_DMRG* Python function is designed to apply the infinite DMRG algorithm to the transverse-field quantum Ising model.
The function takes parameters such as the transverse field strength h, the maximum number of DMRG steps *max_num_steps*, convergence tolerance *tol*, and the coupling strength J. The quantum Ising model is initialized with a single site as the initial system.
The algorithm involves iterative DMRG steps. In each iteration, the function constructs left and reflected enlarged block Hamiltonians along with their interaction terms. These components are used to assemble a superblock Hamiltonian, from which the ground state is obtained. The reduced density matrix of the left block is computed and diagonalized, with the two largest eigenvalues and associated eigenvectors used for truncation. The Hamiltonian is then projected onto this truncated basis, updating the block Hamiltonian and interaction terms.
The iterative process continues until convergence is achieved, determined by a change in energy falling below a specified tolerance, or the maximum number of steps is reached. The function returns the energy per site e, the number of sites N, and the truncation error *truncated_weight*. Specifically, the truncation error is calculated as the sum of the eigenvalues of the reduced density matrix that are excluded during the truncation process. This provides a measure of how much information is omitted in the approximation, with a smaller truncation error indicating a more accurate representation of the quantum state.

2.3 Results

We used the same magnetic field magnitude interval as in the preceding section and employing a convergence tolerance of $\delta = 10^{-8}$.
Figure 5 illustrates a comparison of results obtained from the RSRG and the Infinite DMRG. Observations from the figure indicate that, for $h = 0$, the DMRG method outperforms the RSRG approach. This superiority is particularly evident as, for large N, the DMRG predicts a ground energy per spin e close to the theoretical limit of $-(N-1)/N \simeq -1$. Furthermore, notable discrepancies between the two curves are apparent in the antiferromagnetic region,

highlighting that RSRG overlooks significant terms during the truncation procedure, as previously explained. The larger deviation in the antiferromagnetic regime suggests that the DMRG method provides a more accurate representation, capturing important terms that RSRG neglects.

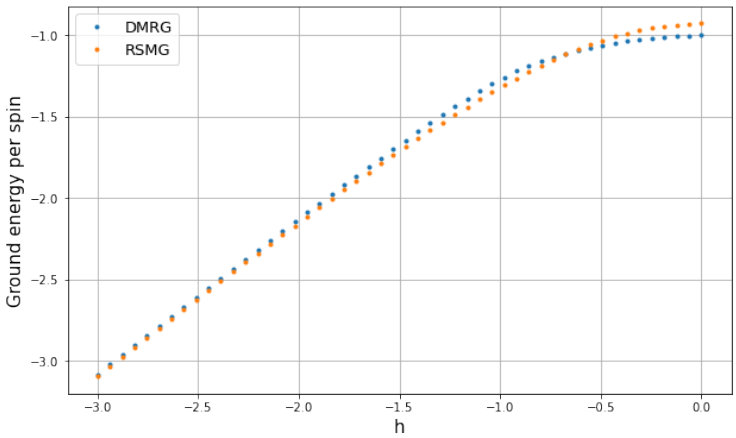

Figure 5: Ground state energy per spin as a function of the magnetic field intensity h. Results for both RSRG and infinite DMRG. The initial system size for the RSRG is $N_0 = 2$, while for DMRG $N_0 = 1$.

In Figure 6, we visualize the average of the sum of neglected eigenvalues in the truncation procedure for different values of h once the convergence is reached, providing insight into the average information omitted in the approximation at each step. The plot reveals an error peak around the phase transition, while for other values of h the approximation is nearly exact. It is noteworthy that this error can be further mitigated by considering an initial system size larger than the one used. However, opting for a larger initial system size increases the computational cost, since the matrix that needs to be diagonalized at each step becomes larger.
Nevertheless, even with the smallest possible initial size (i.e., one site), keeping only the two most significant eigenstates of the reduced density matrix at each iteration, yields a significant approximation, since the peak of the mean error at each step is on the order 10^{-3}.

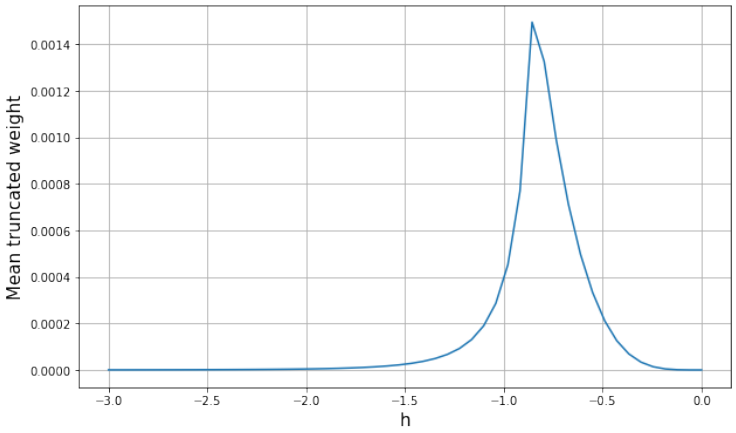

Figure 6: Average of the sum of neglected eigenvalues in the truncation procedure of the infinite DMRG as a function of the magnetic field intensity h.