Assignment 8

Quantum Information & Computing

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Introduction

The **Quantum Ising model** describes a many-body quantum system, which consists of a linear chain of N interacting $1/2$-spins in presence of an external field of intensity λ.

$$\hat{\mathcal{H}} = \Sigma_i^{N-1} \sigma_x^{(i)} \sigma_x^{(i+1)} + \lambda \Sigma_i^N \sigma_z^{(i)}$$

Being it simple but non-trivial, the Ising model is used as a benchmark test for many numerical algorithms.

In this homework we will test two **approximation methods** to study the **thermodynamical limit of many-body quantum systems**.

Real-Space Renormalization Group

Infinite Density Matrix Renormalization Group

Both methods aim to increase the effective size of the quantum system and use a subset of eigenvectors to project in a lower dimensional space without "loosing too much information" on the many-body interactions.

Real-Space Renormalization Group

Init

$$\mathcal{H}^{(0)} = \Sigma_i^{N-1}\, \sigma_x^{(i)}\sigma_x^{(i+1)} + \lambda\, \Sigma_i^{N}\, \sigma_z^{(i)}$$
$$A^{(0)} = \mathbb{1}_{N-1} \otimes \sigma_x$$
$$B^{(0)} = \sigma_x \otimes \mathbb{1}_{N-1}$$

Algo

1. Build the enlarged system Hamiltonian with $2N$ sites:

$$\mathcal{H}_{2N}^{(n)} = A^{(n)} \otimes B^{(n)} + \mathcal{H}^{(n)} \otimes \mathbb{1}_N + \mathbb{1}_N \otimes \mathcal{H}^{(n)}$$

2. Compute the 2^N lowest-energy eigenvectors $|\omega_i\rangle$ of $\mathcal{H}_{2N}$ and let $P = |\omega_i\rangle\langle\omega_i|$.

3. Check the convergence of the energy density $(\varepsilon = \omega_0/2N)$ with a threshold criteria $\Delta_n = |\varepsilon^{(n)} - \varepsilon^{(n-1)}| < \tau$, τ being a target convergence accuracy.

   (?) If the eigenvalue has not converged, get ready for the next iteration,

   - $\mathcal{H}^{(n+1)} \leftarrow \frac{1}{2} \cdot P^\dagger \mathcal{H}_{2N}^{(n)} P$
   - $A^{(n+1)} \leftarrow \frac{1}{\sqrt{2}} \cdot P^\dagger \left(\mathbb{1}_N \otimes A^{(n)}\right) P$
   - $B^{(n+1)} \leftarrow \frac{1}{\sqrt{2}} \cdot P^\dagger \left(B^{(n)} \otimes \mathbb{1}_N\right) P$

   and repeat from (1). Otherwise, return $\varepsilon^{(n)}$.

Infinite Density Matrix RG

Init Let $m_{\max}$ be the maximum allowed size of each left (L) and right (R) block. Initialize the left block L with one site and set

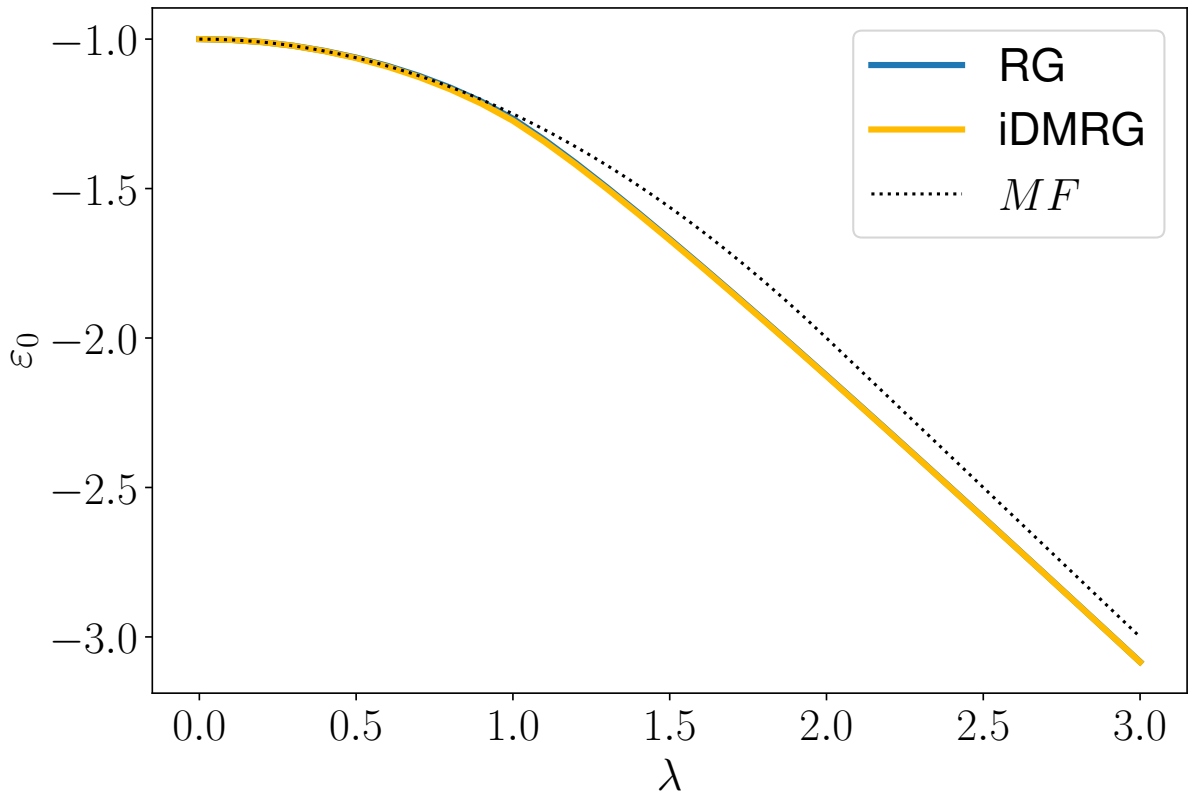
$$\mathcal{H}_L^{(0)} = \lambda\sigma_z \qquad A_L^{(0)} = \sigma_x \qquad B_L^{(0)} = \mathbb{1}_m \qquad m = 1$$

Algo

1. Enlarge the left block by one site $\mathcal{H}_{L+1}^{(n)} \leftarrow \mathcal{H}_L^{(n)} \otimes \mathbb{1}_1 + A_L^{(n)} \otimes \sigma_x + B_L^{(n)} \otimes \lambda\sigma_z$ and update $A_{L+1}^{(n)} \leftarrow \mathbb{1}_m \otimes \sigma_x, \quad B_{L+1}^{(n)} \leftarrow \mathbb{1}_{m+1}$.
2. Build the superblock Hamiltonian $\mathcal{H}^{(n)} = \mathcal{H}_{L+1}^{(n)} + \mathcal{H}_{R+1}^{(n)} + A_{L+1}^{(n)} \otimes A_{R+1}^{(n)}$ and diagonalize it, taking the ground state eigenvector $|\psi\rangle$ and its eigenvalue $\hat{\varepsilon}$.
3. Compute $\rho = |\psi\rangle\langle\psi|$ and trace out the right enlarged block to ρ_{L+1} (reduced density matrix).
4. Diagonalize ρ_{L+1} and build a projector P considering $c = \min(2^m, 2^{m_{\max}})$ eigenvectors associated to the c largest eigenvalues.
5. Project the building blocks for next iteration:
   - $\mathcal{H}_L^{(n+1)} \leftarrow P^\dagger \mathcal{H}_{L+1}^{(n)} P$
   - $A_L^{(n+1)} \leftarrow P^\dagger A_{L+1}^{(n)} P$
   - $B_L^{(n+1)} \leftarrow P^\dagger B_{L+1}^{(n)} P$
6. The energy density is computed at each step as $\hat{\varepsilon}/2(m+1)$.
   ? If not converged, repeat from (1) setting $m = \min(m+1, m_{\max})$.

Results

Benchmarks I have tested Real-Space Renormalization Group with $N = 5, 6, 7$ and the infinite Density Matrix RG with $m_{\max} = 3, 4$. The algorithms have been used to compute the ground state of Ising model in trasverse field probing 30 values of λ equally spaced in $[0, 3]$.



Just for reference, the dotted line is the expected ground state energy density for the thermodynamical limit within the mean field approximation:

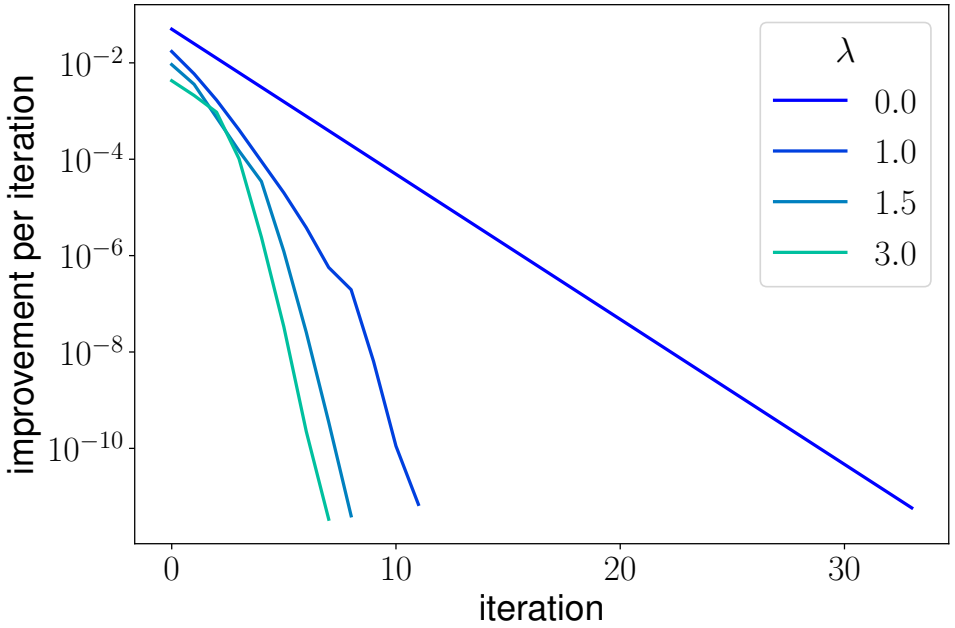
$$\varepsilon_0 = \begin{cases} -1 - \lambda^2/4 & \text{if } |\lambda| < 2 \\ -|\lambda| & \text{else} \end{cases}$$

Results

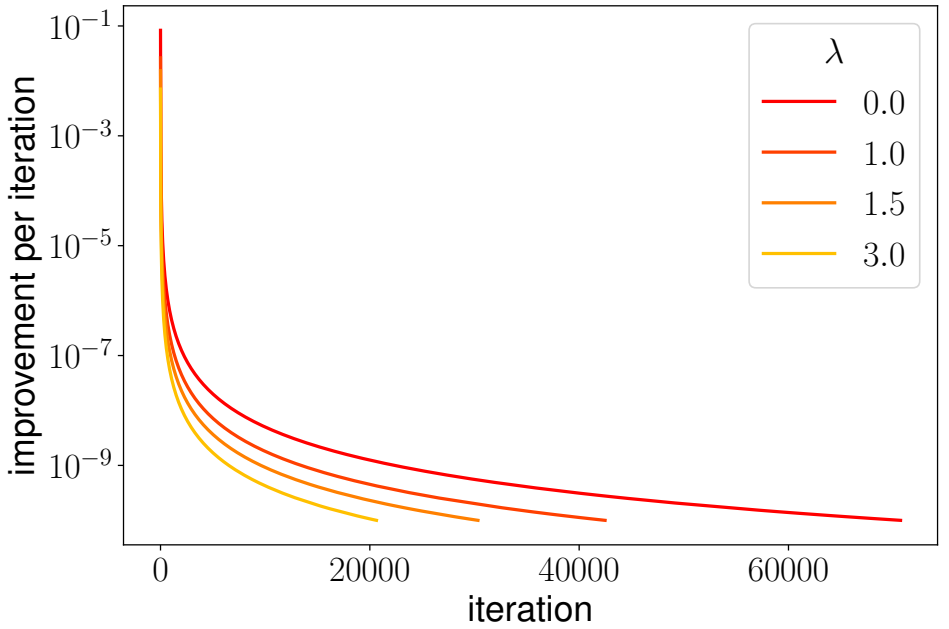
- RG and iDMRG converge both to the same solution.
- RG also converges to the same ground state whatever value of N. Therefore, there is no advantage choosing higher values of N, as the diagonalization of the matrix will take an exponentially longer amount of time.

Results // convergence speed

Even though the algorithms agree on the same solution, their convergence speed is much different.
For instance, we require the algorithms to stop when the system energy converges within $\Delta < 10^{-10}$:



RG converges in a few iterations...



... **iDMRG** takes thousands of iterations.

This behaviour is not unexpected: RG grows the system size exponentially at each iteration, whereas iDMRG increases the number of systems by 2 (so the system grows linearly at each iteration). Nevertheless, this is a price we are willing to pay in case the target physical system violates the underlying assumptions of RG (ex: free particle in a box).