QUANTUM INFORMATION AND COMPUTING

Assignment 7

Author
Marco Chiloiro
December 19, 2023

Transverse-field Ising model

This report looks into the *transverse-field Ising model*, a quantum version of the classic Ising model. We aim to figure out the eigenvalues of the Hamiltonian, which describes the system. We will explore this for different populations of spins and magnetic field strengths.

Theoretical background

Consider a one-dimensional lattice comprising N sites, with each site hosting a spin of one-half. The spins interact exclusively with their immediate neighbors, forming a ring due to periodic boundary conditions. The interaction strength, which depends on the spin projection along the x axis, is determined by a coupling constant J. Additionally, each of the N spins experiences an external magnetic field of uniform intensity h along the z axis. The corresponding Hamiltonian is expressed as:

$$\hat{H} = J\left(\sum_{i=1}^{N-1}\sigma_i^x\sigma_{i+1}^x + \sigma_N^x\sigma_1^x\right) + h\sum_{i=1}^{N}\sigma_i^z, \tag{1}$$

where σ_i^x and σ_i^z denote operators measuring spin along the x and z axes, respectively, for the spin at the i-th position on the lattice ($i = 1, .., N$). These operators, along with the Hamiltonian, operate within a Hilbert space of dimension 2^N. They can be represented as tensor products of operators acting on 2-dimensional Hilbert spaces associated with individual spins, given by:

$$\sigma_i^{x,z} = \mathbf{I}_1 \otimes ... \otimes \mathbf{I}_{i-1} \otimes \sigma^{x,z} \otimes \mathbf{I}_{i+1} \otimes ... \otimes \mathbf{I}_N, \tag{2}$$

where $\mathbf{I_j}$ represents the identity operator acting in the Hilbert space of the j-th spin.
For the analysis, let's set $J = 1$. Given that $J > 0$, the system is antiferromagnetic. In the absence of an external magnetic field ($h = 0$), the ground state is expected to be a superposition of states where neighboring spins are oppositely aligned. Due to entanglement, the mean-field approximation is not applicable in this scenario.
Analogous to the classical case, an increase in the external magnetic field h should induce a phase transition from a antiferromagnetic to a paramagnetic state. This transition occurs as the spins tend to anti-align with the magnetic field to minimize energy. To quantify this behavior, we can compute the average magnetization of the ground state $|\psi_G\rangle$, given by

$$M[\psi_G] = \frac{1}{N}\sum_{i=1}^{N}\langle\psi_G|\sigma_i^z|\psi_G\rangle. \tag{3}$$

By studying the behavior of $M[\psi]$ as the magnetic field intensity varies, we gain insights into the system response to external magnetic influences and the occurrence of the anticipated phase transition from a antiferromagnetic to a paramagnetic state.

Implementation

We implemented a Python function that, given the values of N, h, and J, returns the transverse-field Ising Hamiltonian (1). One can choose the output as a sparse matrix or a

dense matrix by setting a boolean parameter. This function is then imported into the main file, where we use it to recover results and plot the system analysis.
To find the eigenvalues of the Hamiltonian, we utilized two different approaches. When working with sparse matrices, we used the Python function `scipy.sparse.linalg.eigs`, while with dense matrices, we used `numpy.linalg.eigvalsh`. Operating with sparse matrices is computationally more efficient, but it has limitations on computing all eigenvalues. To study the entire spectrum and the degeneracy of the Hamiltonian, we used dense matrices. In this case, the number of elements to store, given the number of spins N, is equal to 2^{2N}. If the elements to store are double-precision reals, the maximum value of N that our computer can manage is $N_{\max} = 13$. Beyond this point, the amount of RAM needed just to store the dense Hamiltonian surpasses about 2 GB for $N = 14$. For larger systems ($N = 14$ and beyond), we used sparse matrices, allowing us to manage Hamiltonians corresponding to systems with up to $N = 20$ spins.
To roughly find the critical point marking the shift from antiferromagnetic to paramagnetic behavior, we used the `numpy.gradient` function in Python. It's worth noting that this method has an error proportional to $O(dh^2)$, with dh being the step size in discretizing the magnetic field intensity h. Essentially, this allowed us to estimate the second derivative of the average magnetization concerning changes in the magnetic field intensity h.
The analysis covers systems with $N \in [3, 10]$, $h \in [-3, 0]$, and $J = 1$ (antiferromagnetic systems).

Results

In Figure 1, the ground state energy per spin is depicted as a function of the magnetic field intensity, h, for various values of N. An interesting observation emerges regarding the fluctuation in ground state energy per spin based on the parity of N, particularly noticeable when $|h|$ is small. Specifically, for small $|h|$, the energies associated with odd N are larger than those associated with even N, which are consistently equal. This distinction arises due to the impact of periodic boundary conditions, introducing frustration in ground states for systems with an odd number of spins. As N increases, the energy per spin difference between systems with even and odd N diminishes, since the frustration energy term is influenced by only one pair of spins. On the contrary, as $|h|$ increases, we observe the disappearance of distinctions between odd and even systems. In this regime, the spins tend to align with each other, leading to the elimination of the frustration term.

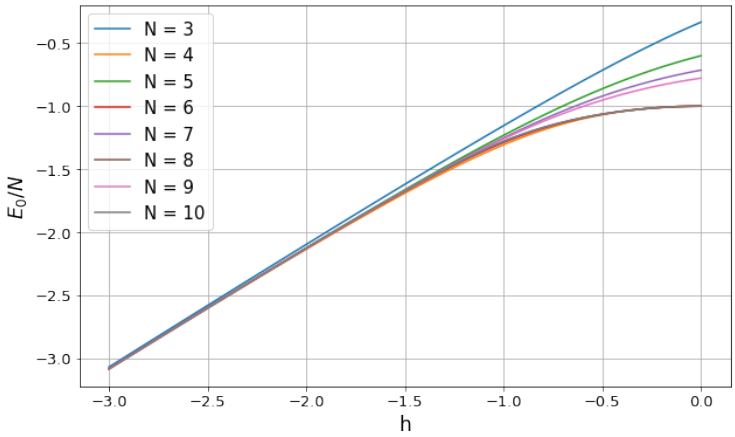

Figure 1: Ground state energy (E_0) per spin (E_0/N) as a function of the magnetic field intensity h, for various numbers of spins N.

For the case when the external magnetic field h is set to zero, the system exhibits antiferromagnetic behavior, where the ground state is characterized by a superposition of states with oppositely aligned neighboring spins. Figure 2 illustrates the average magnetization, defined in (3), as h varies, indicating a second-order phase transition to a paramagnetic state as the magnetic field intensity $|h|$ becomes sufficiently large. To emphasize this transition, we include the second derivative in the plot. The point where the second derivative changes sign serves as an estimate for the critical point of the transition. This extra detail improves our comprehension of how the system behaves in the presence of an external magnetic field. In particular, we can see that the phase transition occurs for h around 1, i.e. for $h \simeq -J$.

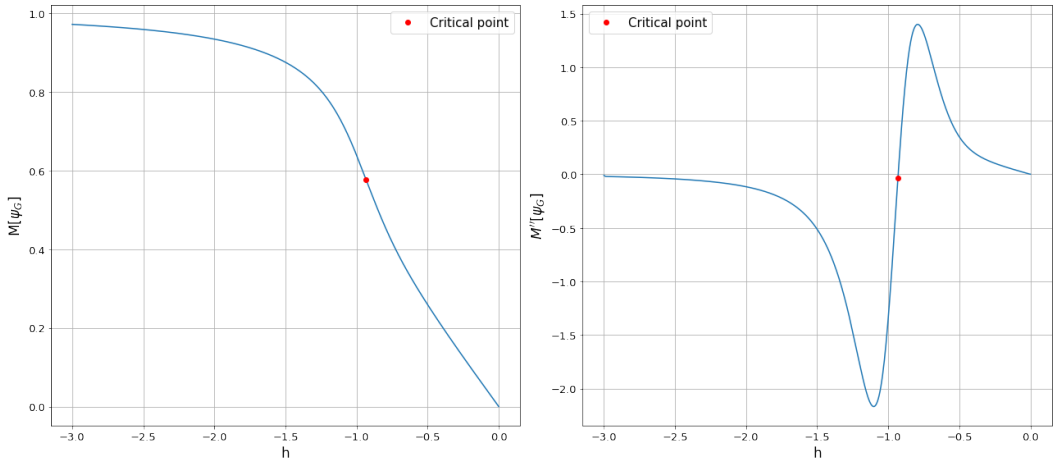

Figure 2: Average magnetization $M[\psi_G]$ as a function of magnetic field intensity h of the ground state of a system composed by $N = 10$ spins, illustrating a second-order phase transition from antiferromagnetic to paramagnetic behavior. The included second derivative helps identify the critical point of the transition.

Finally, we demonstrate that the introduction of a non-zero magnetic field eliminates the degeneracy observed in the excited states. In Figure 3, we present the eigenvalues for

a system consisting of $N = 10$ spins under two different conditions: one with $h = 0$ and the second with $h = -2$. In the first scenario, six energy levels are observed, starting with the ground state where neighboring spins are oppositely aligned. The second level involves three aligned spins, constituting a degenerate state with multiple possible configurations, and so on until reaching situations where all spins are aligned. However, the introduction of a magnetic field, specifically $h = -2$, serves to (partially) break this degeneracy in the energy levels, reducing the energy gap between different levels.

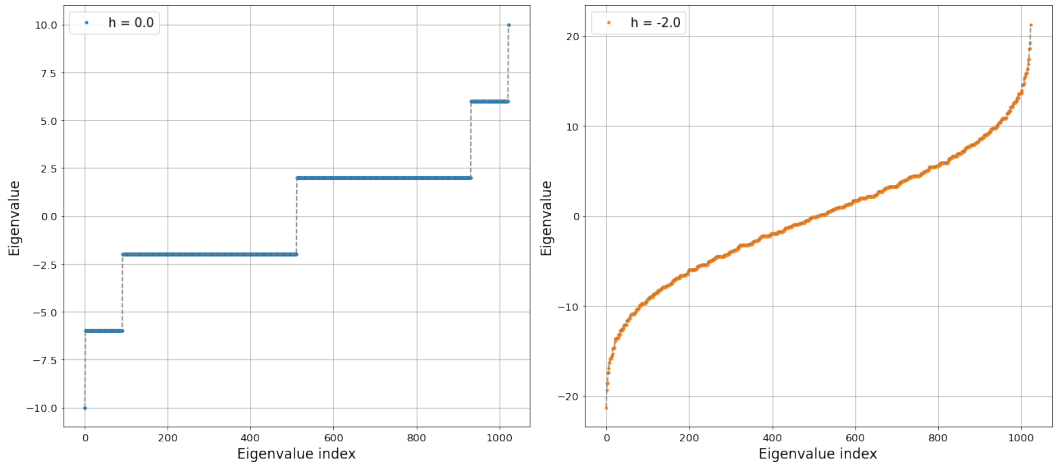

Figure 3: Eigenvalue spectrum of a system with $N = 10$ spins, comparing two scenarios: one with $h = 0$ (on the left) and the other with $h = -2$ (on the right). The eigenvalue indexes correspond to ascending sorted eigenvalues.