Quantum Ising Model

Assignment 7

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Abstract

The quantum Ising model provides a fundamental framework for studying many-body quantum systems. This report investigates a one-dimensional lattice of spin-$\frac{1}{2}$ particles, focusing on constructing the Hamiltonian, diagonalizing it to determine eigenvalues and eigenvectors, and analysing the energy spectrum's dependence on system size and external field strength (λ). By leveraging numerical methods, we explore the interplay between particle interactions and external fields, revealing the system's transition between paramagnetic and ferromagnetic phases. Computational limitations are discussed, with practical constraints restricting the maximum number of particles (N_{max}) to 12. The results demonstrate clustering, crossings, and avoided crossings in the energy spectrum, highlighting the intricate behaviour of quantum systems under varying external fields and interaction strengths.

Introduction

The quantum Ising model is one of the simplest non-trivial many-body quantum systems. It is a simple yet powerful tool to study interacting quantum systems, that exhibits a rich array of phenomena, making it an ideal model for studying quantum phase transitions and many-body quantum states. Spin-$\frac{1}{2}$ systems, which form the basis of the quantum Ising model, are fundamental building blocks in quantum mechanics. These systems are represented as two-level quantum states, commonly referred to as "up" $|\uparrow\rangle$ and "down" $|\downarrow\rangle$, with applications ranging from magnetic materials to qubits in quantum computing. The interactions between these spins, as well as their response to external fields, reveal insights into the collective behaviour of quantum systems.

In this report, the focus is on constructing the Hamiltonian, diagonalizing it to obtain its eigenvalues and eigenvectors, and analysing how these quantities depend on the system size and the external field strength.

Methodology

Formalism

To study the quantum Ising model, we consider N spin-$\frac{1}{2}$ particles on a one-dimensional lattice, that are described by the Hamiltonian $\hat{H}$:

$$\hat{H} = \lambda \sum_i^N \sigma_i^z + \sum_i^{N-1} \sigma_i^x \sigma_{i+1}^x$$

where :

- N is the number of particles,
- λ is the strength of the external field,
- σ_i^z and σ_i^x are the Pauli matrices acting on the i-th particle, i.e.

$$\sigma_i^z = I_1 \otimes I_2 \otimes ... \otimes \sigma_i^z \otimes I_{i+1} \otimes ... \otimes I_N \quad (1)$$

and

$$\sigma_i^x \otimes \sigma_{i+1}^x = I_1 \otimes I_2 \otimes ... \otimes \sigma_i^x \otimes \sigma_{i+1}^x \otimes I_{i+2} \otimes ... \otimes I_N \quad (2)$$

with I_i the identity matrices and the Pauli matrices are :
$\sigma^z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$; $\sigma^x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$

The first term σ_i^z describes the interaction of each spin with the external field, which aligns spins in the z-direction, while the second term $\sigma_i^x \sigma_{i+1}^x$ describes the interaction between neighbouring spins, favouring alignment in the x-direction.

Implementation

In order to numerically implement this formalism, we need first to define the Pauli and identity matrices, σ^z = `sigma_z`, σ^x = `sigma_x` and I = `identity`, as described previously, as well as a function `tensor_product_operators` that takes as inputs a list of operators (represented by 2×2 matrices) and returns the tensor products of these operators.

To compute the matrix representation of the Hamiltonian H, we define the function `hamiltonian(N, S)` that takes as inputs `N`, the number of spin-$\frac{1}{2}$ particles, and `S`, the strength of the external field (λ). It first initializes with zeros a matrix of size $2^N \times 2^N$ (since $\hat{H}$ is a tensor product of N 2×2 matrices). The function first fills the matrix with all the N terms related

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to the external field, and then adds all the N terms related to interaction between the particles, using the function `tensor_product_operators` in order to compute the operators described in equations 1 and 2.

To diagonalize $\hat{H}$, we implement the function `diagonalize_H(H)`, that uses the built-in function `linalg.eigh()` from the NumPy package, to return `eigenvalues` and `eigenvectors`.

Finally, in order to diagonalize $\hat{H}$ for $\lambda \in [-3, 0]$ and plot the first k levels of energy, each time for different values of N, we implement the function `plot_spectrum(N_list, lambda_range, k_levels)` that takes as inputs :

- `N_list`, the list of the different N values to consider,
- `lambda_range`, the array of the values of λ to consider for the computation,
- `k_levels`, the number of energy levels to plot.

Then, for each N, this function will create the Hamiltonian for each λ in `lambda_range` and diagonalize it, with `hamiltonian(N, S)` and `diagonalize_H(H)`, to finally plot the first `k_levels` levels of energy.

Results

N_{max}

The elements of the $2^N \times 2^N$ Hamiltonian $\hat{H}$ are stored as a NumPy array of type `complex`. Python stores `complex` elements as two 64-bit floating-point numbers : 8 bytes for the real part and 8 bytes for the imaginary part. Therefore, each element of $\hat{H}$ has a size of 16 bytes. The total size needed to store all the elements of the matrix representation of the Hamiltonian is $16 \times 2^N \times 2^N = 16 \times 4^N$ bytes, or $\frac{16}{10^9} 4^N$ gigabytes. The code was executed on my personal laptop with 16 GB of RAM. Assuming that all the RAM is free to be used by the code execution, and that the elements will only be stored onto the RAM and not on other types of internal memory storage, we can deduce the theoretical value of N_{max} :

$$\frac{16}{10^9} 4^N \leq 16$$

$$4^N \leq 10^9$$

$$N \leq log_4(10^9)$$

and $log_4(10^9) \approx 14,95$. Theoretically, we have $N_{max} = 14$.

In practice, the code was executed only in a few seconds for $N = 10$, and near a minute for $N = 12$. Above that, it seems that N became too big for $\hat{H}$ to be stored in the RAM, and the execution of the code above $N = 12$ was voluntarily interrupted as too long. This may be due to the fact that not all of the 16 GB of RAM was available, as the operating system and other tasks were using it too. The data may have been temporarily stored onto the internal storage of the computer (SSD), increasing considerably the execution time. In practice, $N_{max} = 12$.

Energy levels

The energy levels of the system depending on the value of $\lambda \in [-3, 0]$ are represented for $N = 1, 2, 3$ and 4 in the figure 1 and for $N = 5$ to 12 in the figure 2.

For the first values of N, a symmetry of the energy levels around 0 can be observed. Indeed. For $N = 1$, there are only 2^1 levels of energy, each of them depending on the parity of the spin as there is no interaction with other spins. For $N = 2$, there are $2^2 = 4$ levels of energy, still symmetric, as the term $\sigma_i^x \sigma_{i+1}^x$ is beginning to influence the interactions between spins but still in a balanced way. From $N = 3$, more complex structures appear, with clustering, crossing and avoided crossing of the energy levels depending on λ.

More generally, it seems that increasing $|\lambda|$, i.e. $\lambda \to -3$, is making the degenerate levels of energy become non degenerate. Indeed, the stronger is the external field, the more broken is the symmetry of the system. When $\lambda \to 0^-$, the system is not perturbed by the external field and the energy levels remain degenerate. Moreover, as N grows, there are more interactions between the N particles, leading to a more complex system with complex interactions between all subsystems. Due to that, the bigger is N, lower are the energy levels.

As λ varies, the system transitions between the paramagnetic phase (aligned along z), with energy levels splitting more evenly due to strong alignment, and ferromagnetic phase (aligned along x), where energy levels reflect this alignment due to the strong coupling between the particles.

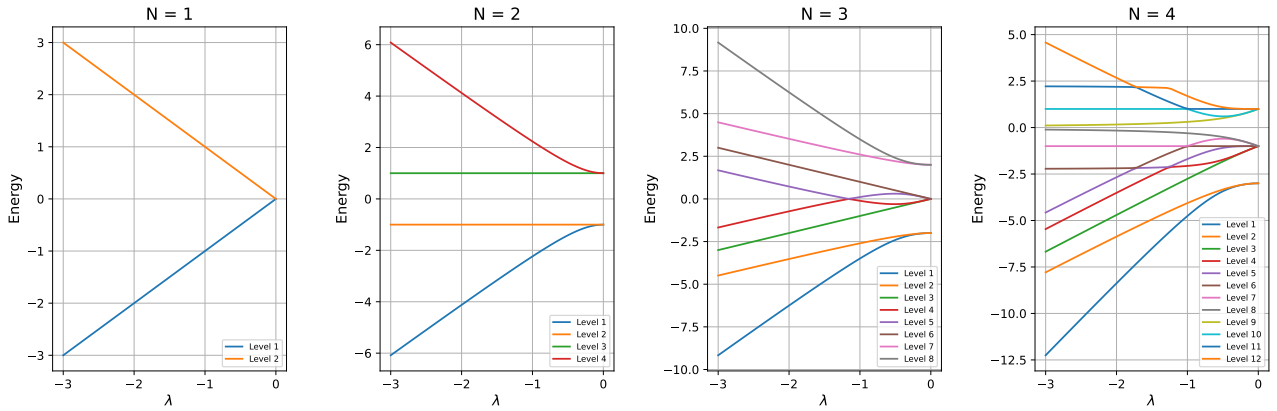

Figure 1: *First 12 levels of energy depending on* λ *for* $N = 1, 2, 3$ *and* 4

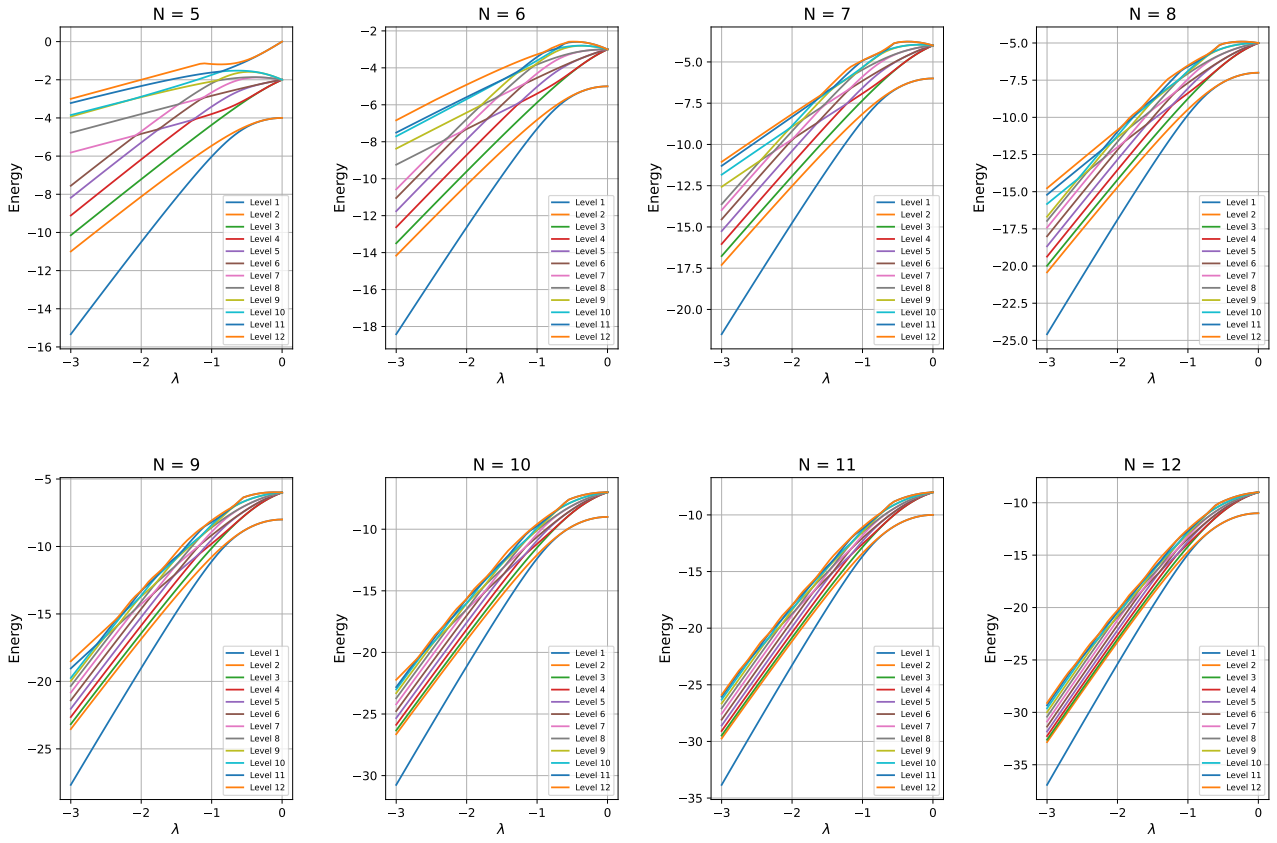

Figure 2: *First 12 levels of energy depending on* λ *for* $N = 5$ *to* 12

Conclusion

The study of the quantum Ising model highlights the rich and complex behaviour of many-body quantum systems. By constructing and diagonalizing the Hamiltonian for systems of up to 12 spin-$\frac{1}{2}$ particles, we observed the intricate evolution of energy levels as a function of the external field strength (λ). For small $|\lambda|$, the energy levels remain degenerate due to the symmetry of the system, while increasing $|\lambda|$ breaks this symmetry, leading to non-degenerate levels and a transition between paramagnetic and ferromagnetic phases. The computational results underscore the limitations imposed by memory and execution time, restricting practical calculations to $N \leq 12$ on standard hardware. This work provides valuable insights into the behaviour of quantum systems and the computational challenges associated with scaling these analyses. Future research could explore optimized algorithms or approximations to extend these calculations to larger systems.