Assignment 7

Quantum Information & Computing

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Theory // Quantum Ising Model in Transverse Field

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.

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

the notation $\sigma_x^{(i+1)}$ contracts $\mathbb{1}_1 \otimes ... \otimes \mathbb{1}_{i-1} \otimes \sigma_x \otimes \mathbb{1}_{i+1} \otimes ... \otimes \mathbb{1}_N$.

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

Using a Mean Field (MF) approach - therefore on the ansatz $|\Psi_{MF}\rangle = \otimes_i^N |\psi_i\rangle$ - the energy density $\varepsilon_0 = E_0/N$ of the ground state of Ising model would be roughly, at the limit $N \to \infty$,

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

Even though this formula is not exact, it encodes a meaningful physical behaviour: the discontinuity of the second derivative in $\lambda = 2, -2$ implies a **quantum phase transition**.

Task

In this homework, we tackle the Quantum Ising model using a "direct" approach.

1. We explicitly build $\hat{\mathcal{H}}$ for finite N and given λ
2. We **diagonalize** $\hat{\mathcal{H}}$, taking the first k eigenvalues and eigenvectors
3. We repeat for different values of λ, sampling in the interval $\lambda \in [0, 3]$

The main computational problems are:

- $\hat{\mathcal{H}}$ is a symmetric matrix of real (double precision) values, of size $2^N \cdot 2^N$. Therefore, the number of elements scales exponentially in N. For instance, in the case of $N = 15$ it would require ~ 8 GB of RAM to store the matrix as `real*8` values. Scaling up to $N = 16$ would require ~ 32 GB of RAM.
- Diagonalization is the most time-consuming step, as it scales exponentially in N, too.

Optimizations // Packed storage and inplace tensor products

These optimizations came to my mind:

- In order to gain a factor 2 on the storage requirement, we can store the Hamiltonian in (upper triangular) packed format, as it is symmetric.

  $\Rightarrow$ The scaling is still exponential, but reduced by a factor 2. An Hamiltonian for $N = 15$ would require ~ 4 GB of RAM.

  All the mathematical operations have to be implemented for upper triangular matrices. For instance, what about the tensor product operations $\otimes$ required to build $\hat{\mathcal{H}}$?

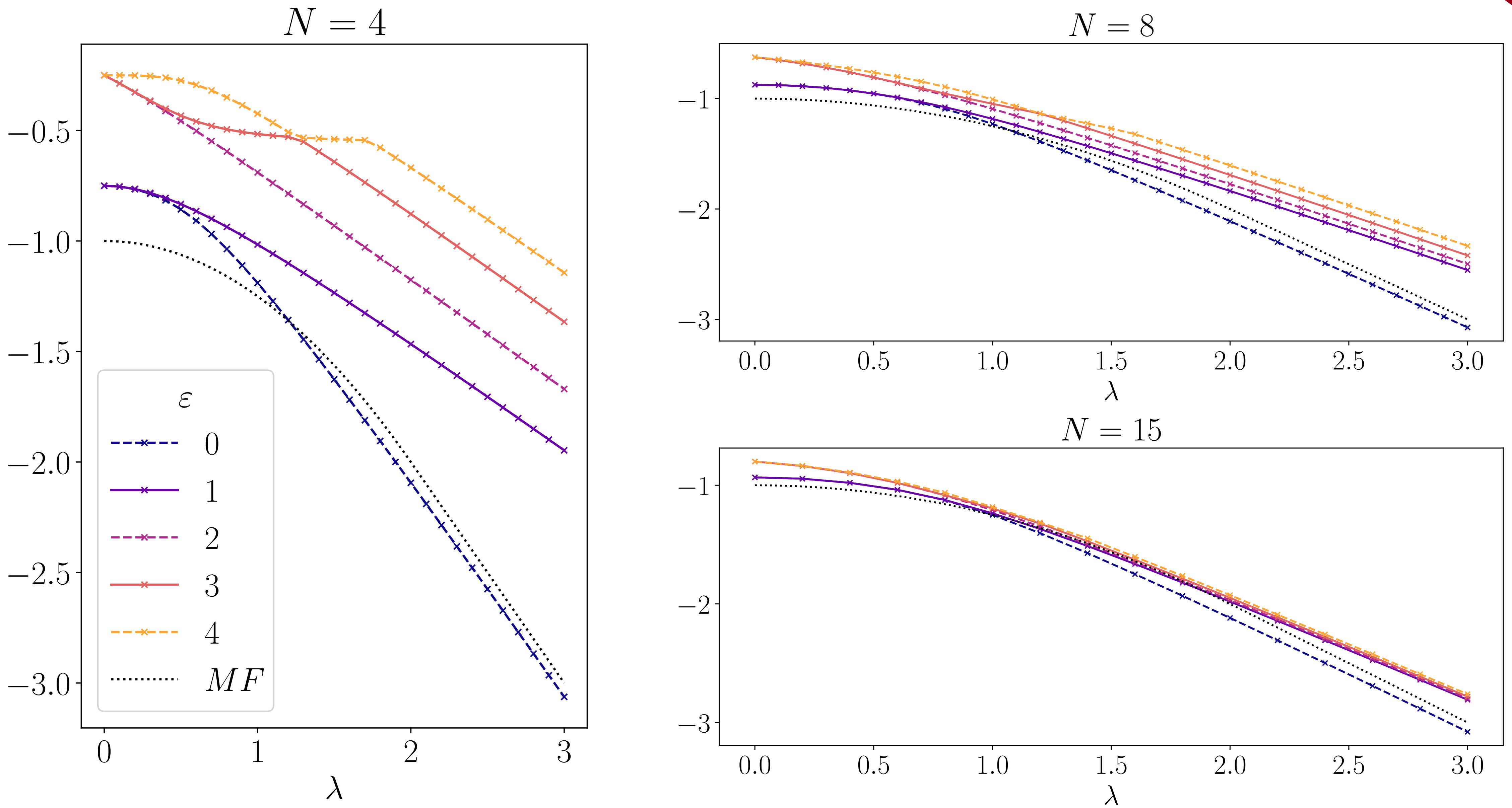
- To make the diagonalization virtually faster, I have used LAPACK with optimized multicore routines from OpenBLAS. Even though the algorithm still scales exponentially, the new backend makes the computer work in parallel with more cores...

To solve the issue ( ), I have implemented routines for **tensor product of upper triangular matrices** ($A \otimes B \leftrightarrow$ `kronp(A,B)`) with **inplace sum** as further optimization; i.e. the chain of operations

$$C \longleftarrow \texttt{kronp(A,B)} + C$$

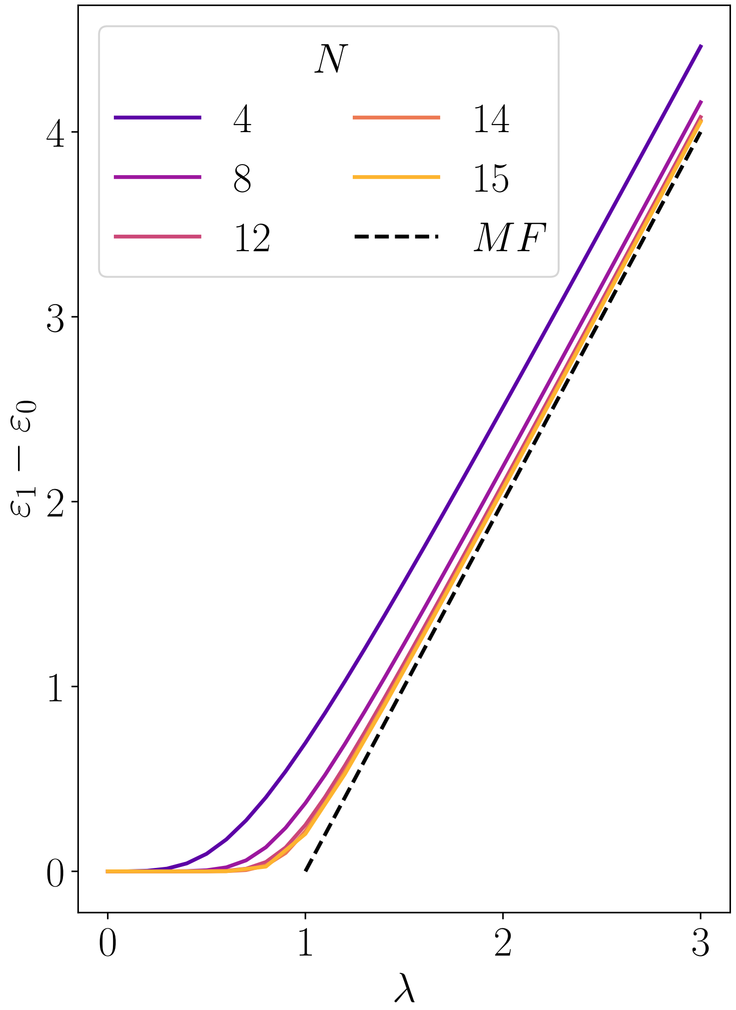
will not require the intermediate storage of the matrix `kronp(A,B)`. Eventually, I optimize with specific routines the tensor products with **left and right identities**: `kronp_l1(n, X)` (for $\mathbb{1}_n \otimes X$) and `kronp_r1(X, n)` (for $X \otimes \mathbb{1}_n$).

Results // Energy **density** spectrum for N spins

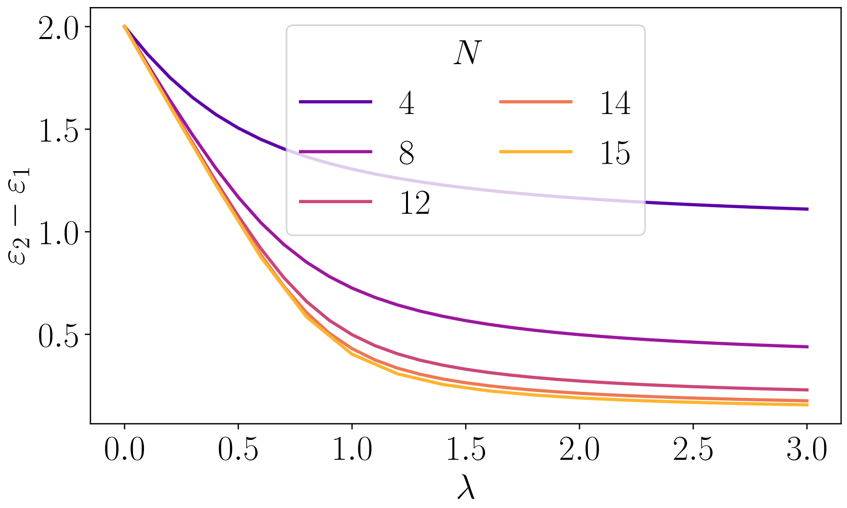


Results // Energy gap

Another interesting perspective on the Ising problem is the **energy gap between the ground state and the first two excited levels** ε_1 and ε_2.



- In the area of stronger external field $|\lambda| > 1$, known in literature as **disordered phase**, we observe that systems with more spins (larger N) have ground-state energy closer to the theoretical limit in MF theory.
- In the regime $0 < |\lambda| < 1$ the system is said to be in **ordered phase**, and the gs breaks the spin-flip symmetry.
- For $\lambda \to 0$, all the levels are degenerate, as expected.



The gap between the second excited state and the first excited state

$$\varepsilon_2 - \varepsilon_1 \to 2$$

for $\lambda \to 0$.