Quantum Information and Computing (QIaC)

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Theory

The system we investigated in this assignment is the **transverse-field Ising model** (TFI), which describes a sequence of N spins under the presence of a transverse magnetic field. The Hamiltonian for such a system is the following:

$$\hat{H} = -J \sum_{i=1}^{N-1} \hat{\sigma}_x^i \hat{\sigma}_x^{i+1} + \lambda \sum_{i=1}^{N} \hat{\sigma}_z^i \tag{1}$$

where the $\hat{\sigma}$ are the **Pauli operators**, λ is a coupling constant indicating an **external field** and we set $J = 1$. When we write the interaction term or the single site operator, acting on the whole sequence of spins, what is actually meant is that:

$$\hat{\sigma}_z^i = \mathbb{1}_1 \otimes \cdots \otimes \mathbb{1}_{i-1} \otimes \hat{\sigma}_z^i \otimes \mathbb{1}_{i+1} \otimes \cdots \otimes \mathbb{1}_N \tag{2}$$

$$\hat{\sigma}_x^i \hat{\sigma}_x^{i+1} = \mathbb{1}_1 \otimes \cdots \otimes \mathbb{1}_{i-1} \otimes \hat{\sigma}_x^i \otimes \hat{\sigma}_x^{i+1} \otimes \mathbb{1}_{i+2} \otimes \cdots \otimes \mathbb{1}_N \tag{3}$$

i.e. the Hamiltonian is a **sum over tensor products** of operators (identities and Pauli matrices) acting on all the sites. In the code we are going to **reuse** the double complex matrix `TYPE` defined in week 3. With the newly implemented subroutines and functions we are able to investigate the **spectrum** of the first $k = 4$ eigenvalues, highlighting the behavior of the system near the **quantum critical point** (QCP) at $\lambda = 1$

Two main code snippets

- We report the function to compute the tensor product between two generic matrices (left), and the one for the initialization of the Hamiltonian operator (right). For the former we recall that, being m_1 and m_2 two matrices:

$$m_1 \otimes m_2 = \begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix} \otimes \begin{pmatrix} a_2 & b_2 \\ c_2 & d_2 \end{pmatrix} = \begin{pmatrix} a_1 \cdot a_2 & a_1 \cdot b_2 & b_1 \cdot a_2 & b_1 \cdot b_2 \\ a_1 \cdot c_2 & a_1 \cdot d_2 & b_1 \cdot c_2 & b_1 \cdot d_2 \\ c_1 \cdot a_2 & c_1 \cdot b_2 & d_1 \cdot a_2 & d_1 \cdot b_2 \\ c_1 \cdot c_2 & c_1 \cdot d_2 & d_1 \cdot c_2 & d_1 \cdot d_2 \end{pmatrix}$$

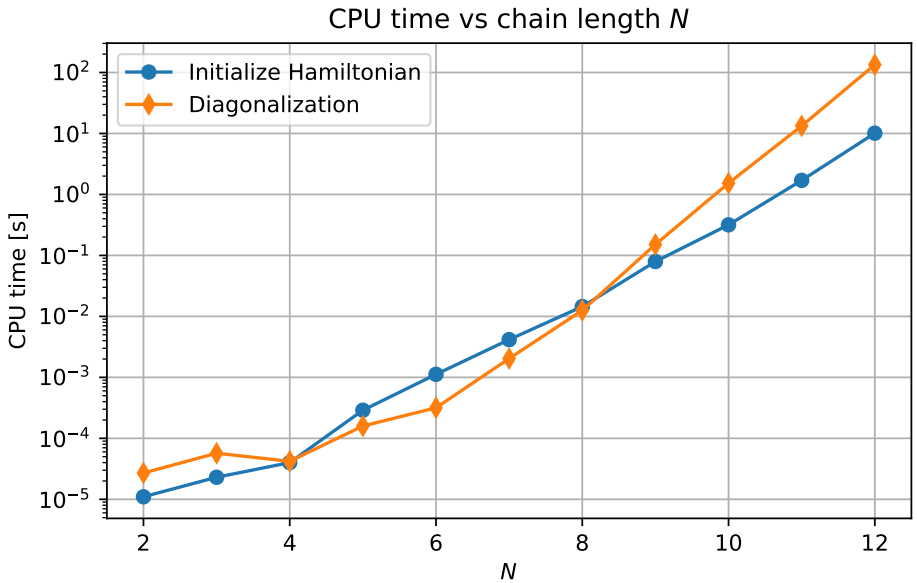
  The indices `ii`, `jj` run over m_1, and we call (`rf`,`cf`) and (`rl`,`cl`) as the indices on the bigger matrix for the output of $m_1(ii, jj) \cdot m_2$.

```
FUNCTION tp(m1 ,m2) RESULT(output)
![...]
ALLOCATE(output(n_row1*n_row2,n_col1*n_col2))
![...]
!cycle on the elements of the first matrix
DO ii = 1, n_row1
    DO jj = 1, n_col1
        !creating indices of the output matrix
        rf = (ii - 1) * n_row2 + 1
        cf = (jj - 1) * n_col2 + 1
        rl = ii * n_row2
        cl = jj * n_col2
        output(rf:rl,cf:cl) = m1(ii,jj)*m2
```

```
FUNCTION TFI_ham_init(N, lambda) RESULT(output)
![...]
DO ii = 1, N
    !single site component
    output = output + tp(tp(id_mat_init(ii-1),
             sigma_z()),id_mat_init(N-ii))
ENDDO
output = output * lambda* COMPLEX(1.0d0, 0.0d0)
DO ii = 1, N-1
    output = output - tp(tp(tp(id_mat_init(ii-1),
    sigma_x()),sigma_x()),id_mat_init(N-ii-1))
```

Results - Efficiency

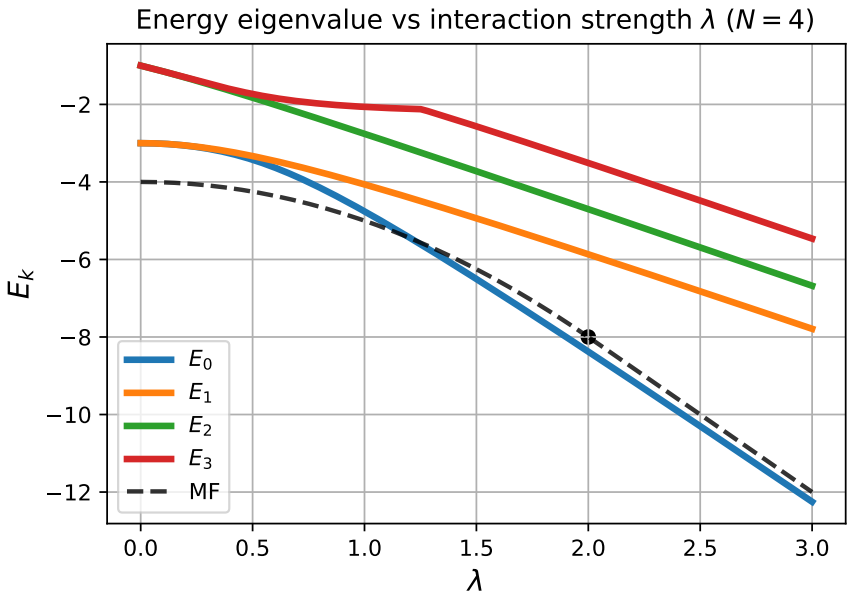
We used several Python **scripts** to **automatize** the work and produce the following graphs. Here we fix $\lambda = 1$ and we study how the **time required** for the initialization of the Hamiltonian, and for the diagonalization routine scales with N.

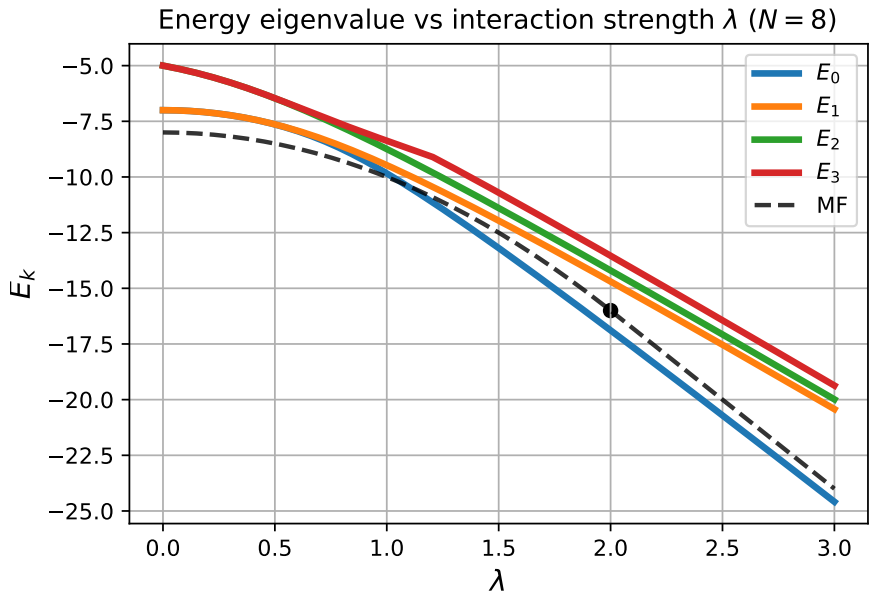


Both of them have an **exponential** behavior, and in particular the diagonalization subroutine requires more time than the initialization of the Hamiltonian. We can surely gain some performances with a better fine tuning of the parameter of the `ZHEEV` subroutine, but we will still have to wait a long time. In the end, this forces us to work with $N < 10$ systems and so to be far away from the behaviors expected in the thermodynamic limit $N \to \infty$.

Results - Energy spectrum

We run the code for $N = 4, 8$, $\lambda \in [0, 3]$, and we plot the first 4 energy eigenvalues, and the results obtainable with a **mean-field** approach (MF): $E/N = 1 - \lambda^2/4$ for $\lambda \in [-2, 2]$ and $E/N = -|\lambda|$ for $\lambda \notin [-2, 2]$.

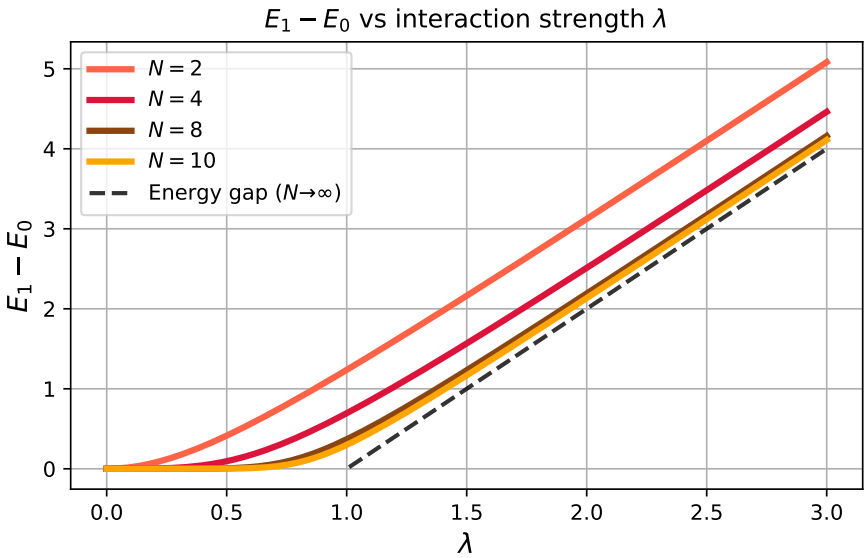


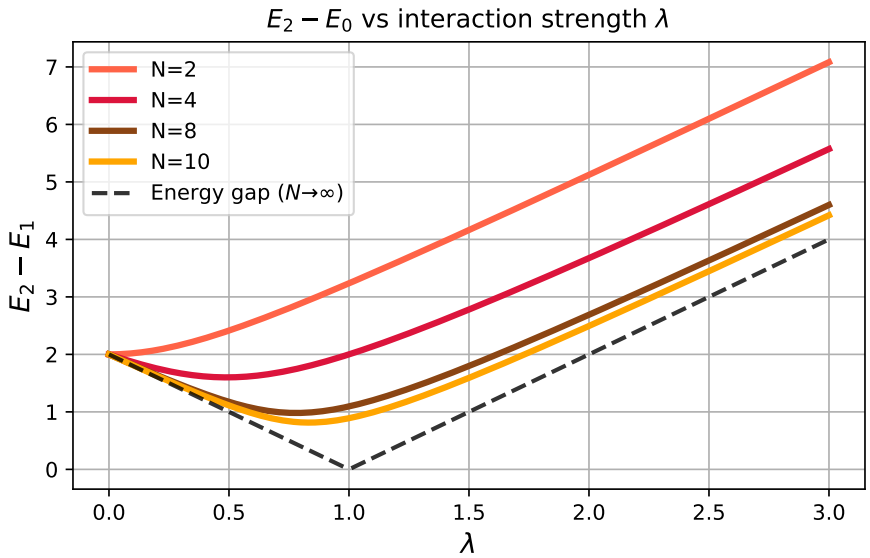


For a **weak field** $\lambda \to 0$ the two energy levels are degenerate, the interaction term is dominating and all the spins are anti-aligned to minimize the energy ($N = 4 : |\uparrow\downarrow\uparrow\downarrow\rangle$ or $|\downarrow\uparrow\downarrow\uparrow\rangle$ and $E = -3$). MF gives a wrong estimate of the GS energy: $-N \langle\psi| \sigma_x |\psi\rangle^2 = -4$, and of the QCP at $\lambda = 2$, rather than $\lambda = 1$. For a **strong field** $\lambda \to \infty$ the external field is dominating, and $E_0 \approx -N\lambda$. Furthermore, we also notice how the energy gap becomes narrower as N increases (comparing it to the left graph). Moreover, the **bifurcation point** (at $\lambda < 1$ in our cases) of the quantum phase transition approaches $\lambda = 1$ for $N \to \infty$.

Results - Energy gap

We plot here the energy gap between the first and the ground state eigenvalue $E - 1 - E_0$, and the one between the lowest excited state and the ground state $E_2 - E_0$.





Taking into account the two graphs of the previous slide, we see how below $\lambda = 1$ (the quantum critical point), the energy difference is 0, since the ground state is **two-folded** (degenerate). The solution approaches the theoretical one in the thermodynamic limit $N \to \infty$.

The lowest excited state E_2 has an energy higher than the ground state E_0 by a nonzero amount (non-vanishing for $N \to \infty$), that is $2(1 - \lambda)$ in the thermodynamic limit for $\lambda < 1$. The energy gap for $\lambda > 1$ and $N \to \infty$ is $2(\lambda - 1)$. The solution approaches the theoretical one in the thermodynamic limit $N \to \infty$.