Presentation of Assignment 7

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Theoretical introduction

We consider a one-dimensional system with N $\frac{1}{2}$ spins, described by the Hamiltonian

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

where σ_x, σ_z are Pauli matrices and λ is the interaction strength. More precisely, a term σ_i^z is a shorthand notation to indicate $\mathbb{I}_{i-1} \otimes \sigma_i^z \otimes \mathbb{I}_{N-i}$, and similarly for the $\sigma_i^x \sigma_{i+1}^x$ terms.

In order to solve the eigenproblem $\hat{H}|\psi_k\rangle = E_k|\psi_k\rangle$, we recast the Hamiltonian (a tensor of rank N) into a $2^N \times 2^N$ matrix that can be solved with well-optimized LAPACK routines. In matrix form, the interaction terms are written as

$$\sigma_i^z = \text{diag}\left(\mathbb{I}_{N-i}, -\mathbb{I}_{N-i}, \underbrace{\ldots\ldots}_{2^{i-1}\text{times}}\right),$$

$$\sigma_i^x \sigma_{i+1}^x = \text{diag}\left(\mathbb{A}_{N+1-i}, \underbrace{\ldots\ldots}_{2^{i-1}\text{times}}\right), \quad \text{with } \mathbb{A}_k = \begin{pmatrix} 0 & & & \mathbb{I}_{k-2} \\ & & \mathbb{I}_{k-2} & \\ & \mathbb{I}_{k-2} & & \\ \mathbb{I}_{k-2} & & & 0 \end{pmatrix}.$$

Code development - Matrix creation

- **Filling of $\sigma_{\mathbf{i}}^{\mathbf{z}}$ terms**: The matrix representation of σ_i^z is diagonal and its elements can be easily computed considering the alternating behavior of the sign. In particular, the j-th diagonal element of σ_i^z is $(-1)^{\left\lfloor (j-1)/2^{N-i} \right\rfloor}$ $\left(\text{for } 1 \leq j \leq 2^N\right)$.
- **Filling of $\sigma_{\mathbf{i}}^{\mathbf{x}}\sigma_{\mathbf{i+1}}^{\mathbf{x}}$ terms**: The matrix representation consists of 2^{i-1} square blocks on the diagonal, denoted as $\mathbb{A}_{N+1-i}$, of length 2^{N+1-i}. The subroutine **fillAntidiag** takes a section of the total matrix and fills it with $\mathbb{A}$. For a given i, this subroutine is called 2^{i-1} times to fill every $2^{N+1-i} \times 2^{N+1-i}$ block on the diagonal.

Subroutine to fill antidiagonal submatrix A (Ising1D.f90)

```
SUBROUTINE fillAntidiag(AA, k)
    ! filling of leftermost identity submatrix
    DO ii = 1, 2**(k-2)
        AA(3*(2**(k-2))+ii, ii) = AA(3*(2**(k-2))+ii, ii) + 1
    END DO

    ! filling of second leftermost identity submatrix
    DO ii = 1, 2**(k-2)
        AA(2*(2**(k-2))+ii, 1*(2**(k-2))+ii) = AA(2*(2**(k-2))+ii, 1*(2**(k-2))+ii) + 1
    END DO

    ! ... filling of second rightermost and rightermost identity submatrices ...
END SUBROUTINE fillAntidiag
```

Code development - Matrix diagonalization

An example of the Hamiltonian computed for fixed N and λ is shown in Figure 1. The nested antidiagonal structure highlighted in red is caused by the $\sigma_i^x \sigma_{i+1}^x$ interaction terms, whereas the diagonal elements are given by the σ_i^z terms.

The LAPACK subroutine **DSYEVX** is used to calculate the first K_{max} eigenvalues of $\hat{H}$. The procedure is repeated for different $\lambda \in [0, 3]$ to obtain the lower energy spectrum of $\hat{H}$ for a given N. The routine is well optimized for the task, so **the biggest limitation is the memory needed to store a $2^N \times 2^N$ double-precision real matrix**.

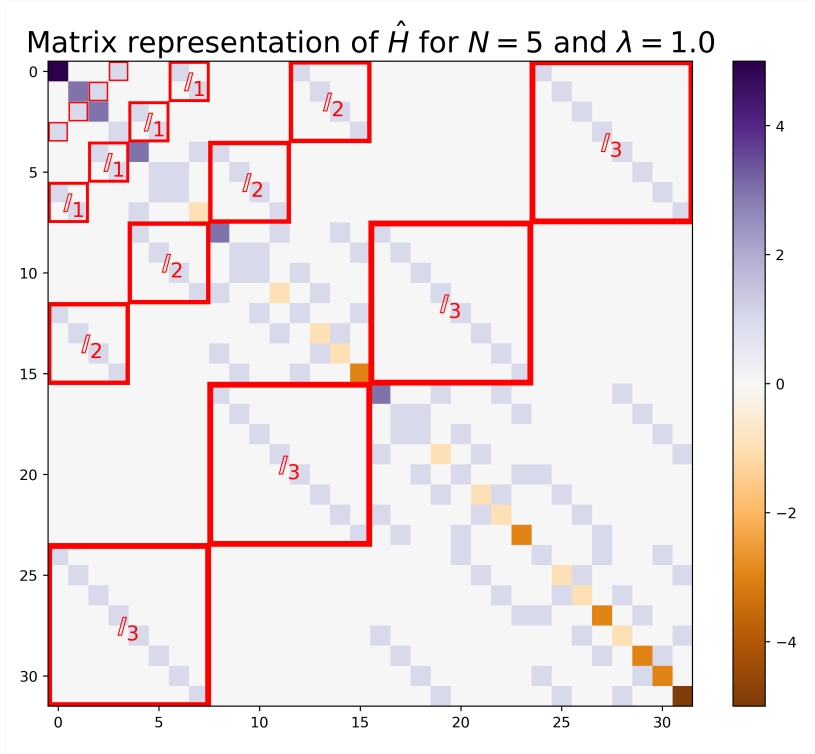
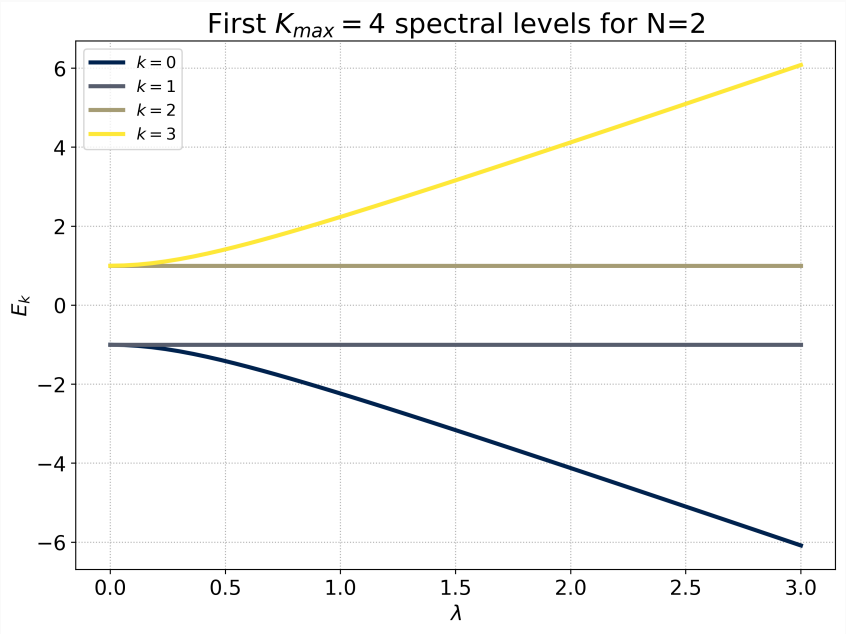


Figure 1: Example of matrix representation of $\hat{H}$

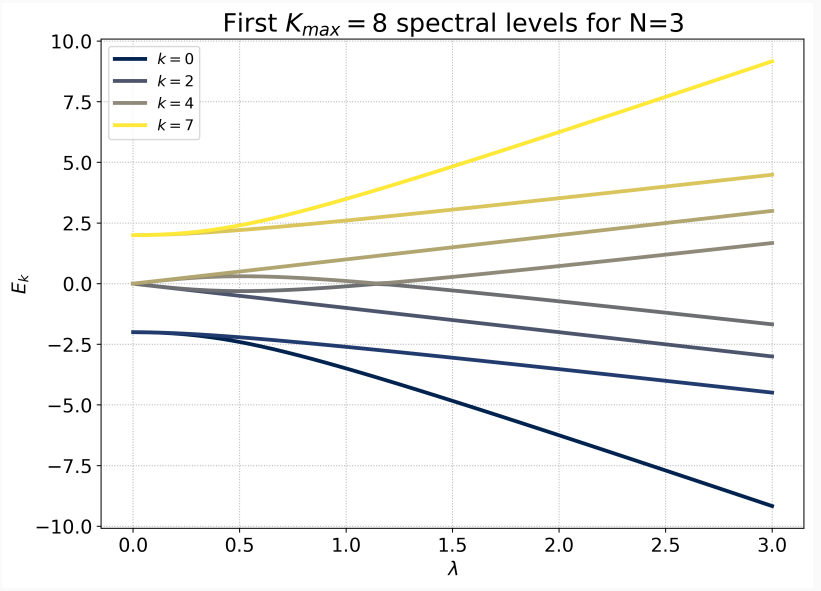
Call to DSYEVX diagonalization subroutine (Ising1D.f90)

```
! call diagonalization routine
CALL DSYEVX('N', 'I', &              ! compute only eigenvalues with index in [IL,IU]
          'L', 2**NN, HN, 2**NN, &   ! store lower triangular matrix of 2**NN x 2**NN matrix HN
          0.D0, 1.D0, &              ! VL, VU are not referenced since RANGE="I"
          1, K_max, &                ! find eigenvalues from IL=1 to IU=K_max
          2*DLAMCH('S'), &           ! absolute error tolerance for the eigenvalues
          eig_num, eigenvals, &      ! eigenvalues and eigenvalues number
          ...)
```

Results - Complete spectra



A common pattern observed in the complete spectra for $N = 2, 3, 4$ is the **degeneracy** of the 2^N energy levels **at $\boldsymbol{\lambda = 0}$** into N energies, the first and last of which have degeneracy $= 2$ for every N. For $\lambda > 0.5$, all energy levels are clearly distinguishable. Moreover, **energy levels are also symmetric w.r.t. $\mathbf{E = 0}$**, so the full spectrum can be obtained from its lower half with $E \leq 0$.



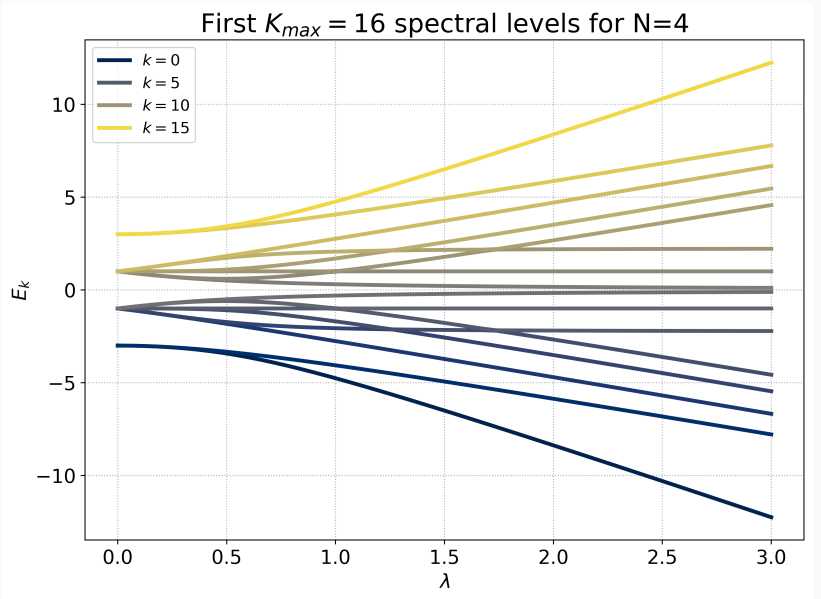


Figure 2: Complete spectra for some values of N

Results - Spectra for high N

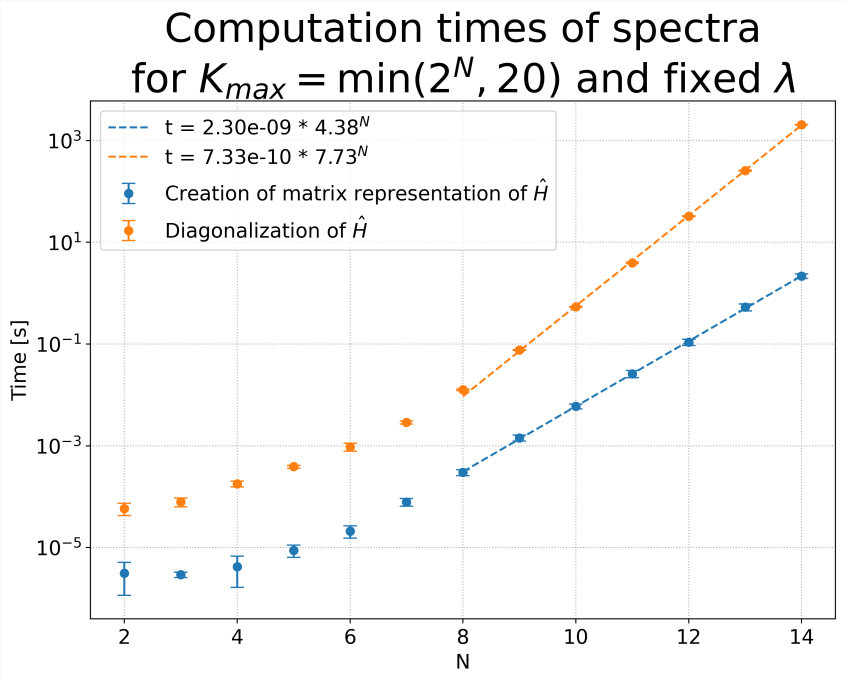


Figure 3: Time-scalings of spectra calculations

Tests performed on an 8GB RAM VM.

The largest value of N for which it was possible to compute the first $K_{max} = 20$ energy levels is $\boldsymbol{N_{max} = 14}$. In fact, $N = 15$ would require 8GB of RAM to store the matrix representation and about 4h 20min to compute $K_{max} = 20$ energies at a given λ.

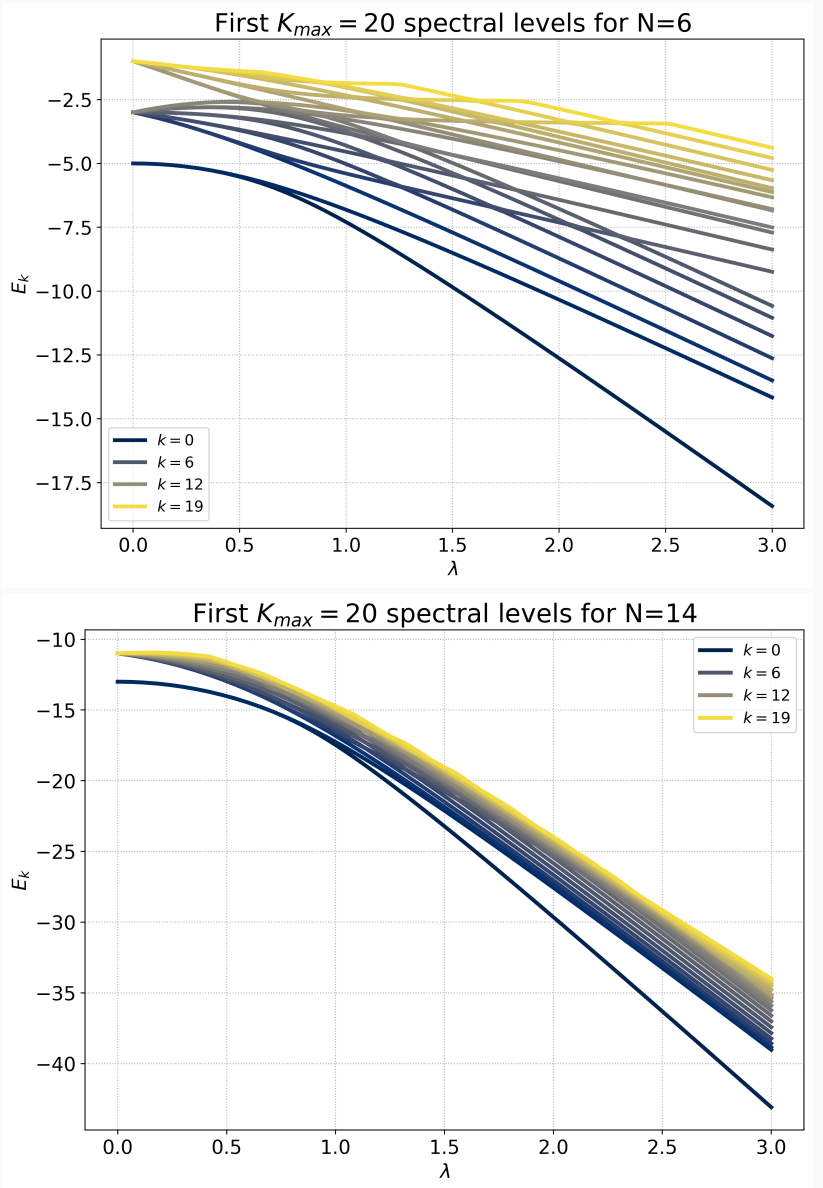


Figure 4: Spectra for some high values of N