Exercise 9: *Numerical evaluation of the Ising Model in* FORTRAN

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Abstract

The N-spin 1/2 **Ising model** on a one-dimensional lattice is consider. The **Hamiltonian** of the model is given by: $H = \lambda \sum_{i=1}^{N} \sigma_i^z + \sum_{i=1}^{N-1} \sigma_i^x \sigma_{i+1}^x$ where σ represents the Pauli matrices and λ the interaction strength. In particular, the first four **eigenenergies** are computed using the LAPACK library, for several N. Finally, the Hamiltonian spectrum is analyzed and a quantum phase transition is found.

1 Introduction

The quantum Ising model is given with the Hamiltonian:

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

where σ are the Pauli matrices and represents a linear chain of N interacting spins 1/2 in presence of an external field of intensity λ. In discussing the Hamiltonian 1, it is convenient to choose a system of basis vectors in which S_i^z is diagonal:

$$\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2}$$

The Hilbert space corresponding to a system of N spin 1/2 atoms is 2^N dimensional. Exact diagonalization of such systems can be quite formidable, even on the fastest computers, due to the exponential increase in the dimensions of the Hamiltonian matrix with increasing N. Nevertheless, since we know the individual spin operator we can construct the composite spin operator by using the tensor product structure of the Hilbert space:

$$\sigma_z^i = \mathcal{I}^1 \otimes \mathcal{I}^2 \otimes \ldots \otimes \sigma_z^i \otimes \ldots \otimes \mathcal{I}^N \tag{3}$$

and the interaction term results in:

$$\sigma_x^i \sigma_x^{i+1} = \mathcal{I}^1 \otimes \mathcal{I}^2 \otimes \ldots \otimes \sigma_x^i \otimes \sigma_x^{i+1} \otimes \ldots \otimes \mathcal{I}^N \tag{4}$$

In order to have a qualitative intuition about what should happen, the mean field solution is presented which is given by:

$$|\Psi^{MF}\rangle = \bigotimes_{i=1}^{N} |\Psi^1\rangle = \bigotimes_{i=1}^{N} \sum_{\alpha_i=1}^{d} A_{\alpha_i} |\alpha_i\rangle \tag{5}$$

Under this assumption, the computation of the system's energy can be done as:

$$E^{MF} = \langle \Psi^{MF} | \mathcal{H}^1 | \Psi^{MF} \rangle = -\sum_{i=1}^{N-1} (\langle \Psi^1 | \sigma_i^x | \Psi^1 \rangle)^2 + \lambda \sum_{i=1}^{N} \langle \Psi^1 | \sigma_i^z | \Psi^1 \rangle \tag{6}$$

Notice that the above quantity is extensive, thus it diverges at the thermodynamics limit, while the energy density $e = E/N$ is intensive, therefore in the thermodynamic limit $N \to \infty$ it holds:

$$E[\psi_{MF}] = \langle \psi_{MF} | H | \psi_{MF} | = \sum_{j=1}^{N-1} \langle \psi_{MF} | \sigma_x^j | \psi_{MF} \rangle^2 + \lambda \sum_{i=1}^{N} \langle \psi_{MF} | \sigma_z^i | \psi_{MF} \rangle \tag{7}$$

The ground state of the system is:

$$e = \begin{cases} -1 - \frac{\lambda^2}{4} & \lambda \in [-2; 2] \\ -|\lambda| & \lambda \notin [-2; 2] \end{cases} \tag{8}$$

The expression above is not exact; however, it captures the physics of the system in the sense that it signals that there are two special points, $\lambda = -2, 2$ where the second derivative of the energy density becomes a discontinuous function.

In this report, the first eigenvalues of the Ising model described before for a system of N spins 1/2 are found. In particular, the limitation arising of the computational complexity due to value N are study.

2 Code development

The most interesting part is to build the Ising Hamiltonian given Equation 1, which is a $2^N \times 2^N$ matrix for a system of N spin 1/2. This was done by building first the magnetic and the interacting part independently. Listing 1 shows the initialization matrix of the magnetic part which is diagonal due to the fact that we have chosen σ_z to be diagonal.

```
! Building diagonal term
hamiltonian_diagonal = 0
do ii=1,n_part
    tmpvar = ham_dim**(n_part+1-ii)
    do jj=0,ham_dim**n_part-1,tmpvar
        hamiltonian_diagonal((jj+1):(jj+tmpvar/2)) = hamiltonian_diagonal((jj+1):(jj+tmpvar/2)
    )+1
        hamiltonian_diagonal((jj+tmpvar/2+1):(jj+tmpvar)) = hamiltonian_diagonal((jj+tmpvar
    /2+1):(jj+tmpvar))-1
    enddo
enddo

   hamiltonian_magentic = 0
do ii = 1, ham_dim**n_part
    hamiltonian_magentic(ii,ii)=hamiltonian_diagonal(ii)
enddo
```

Listing 1. Generation of the magnetic part of the Ising model

The implementation of the interaction part is a little bit more tricky since a tensor product among two matrices that are not diagonal are needed. Moreover, a FUNCTION called `tensor_product` that implements the tensor product among two matrices were built in a different MODULE. In par-

ticular, for the interaction term a loop over the $N-1$ couples was needed. A support matrix `temp` stores the temporary values at each step. The tensor products are evaluate by knowing the first "trivial value" which is either the Pauli matrix or the Identity matrix depending on the position and by using the already mentioned `tensor_product` function. This is shown in Listing 2.

```
!initializing matrix for interaction term
hamiltonian_J = 0
do ii=1,n_part-1
    temp = 0
    do jj=1,n_part
        if (jj==1) then
            if (((n_part+1-jj).eq.ii).or.((n_part+1-jj).eq.(ii+1))) then
                temp(1:ham_dim**(jj),1:ham_dim**(jj)) = sigma_x(:,:) !sigma x
            else
                temp(1:ham_dim**(jj),1:ham_dim**(jj)) = I(:,:) !identity
            endif
        else
            if (((n_part+1-jj).eq.ii).or.((n_part+1-jj).eq.(ii+1))) then
                !perform tensor product
                temp(1:ham_dim**(jj),1:ham_dim**(jj)) = tensor_product(sigma_x, temp( 1:
    ham_dim**(jj-1),1:ham_dim**(jj-1) ))
            else
                temp(1:ham_dim**(jj),1:ham_dim**(jj)) = tensor_product(I, temp( 1:ham_dim**(jj
    -1),1:ham_dim**(jj-1) ))
            endif
        endif
    enddo
    hamiltonian_J(:,:) = hamiltonian_J(:,:) + temp(:,:)
enddo
```

Listing 2. Generation of the interacting part of the Ising model

All the matrices are checked to be Hermitian (recalled that the tensor product among two Hermitian matrices remains Hermitian). Finally, the two matrices are summed together with the interaction parameter λ multiply in the magnetic term. In particular, we loop over λ choosing itself to be linear $\lambda_i = 0 + i(3/20)$. Moreover, the eigenvalues are found by diagonalizing the matrix using an already done preiously week SUBROUTINE that use the `zheev` function provided by LAPACK. The implementation is shown in Listing 3

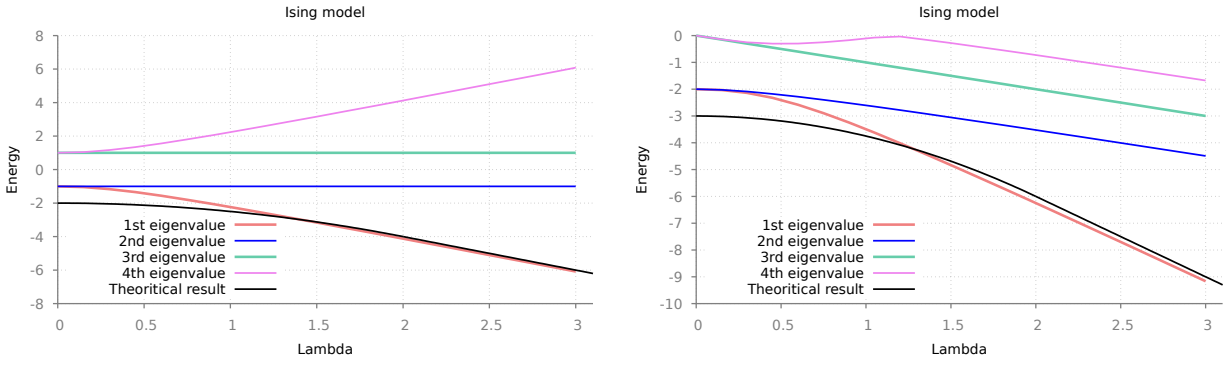
```
do ii = 0, 20
    lambda = 3._pr/(20._pr)*ii
    hamiltonian = 0
    hamiltonian(:,:) = hamiltonian_J(:,:) + lambda *hamiltonian_magentic(:,:)
    call check_hermitian(hamiltonian,debug)
    info =0
    !compute eigenvalues calling subroutine
    call eigenvalues(hamiltonian, ham_dim**n_part, work, eigen, rwork,  lwork, info)
    if(info.NE.0)then
        print*,'DIAGONALIZATION FAILED'
        stop
    end if
```

Listing 3. Main code of SUBROUTINE to generate generic states

All the results are saved in a correspondent file. The FORTRAN program is automated in PYTHON and perform changing the variable N. Furthermore, also the GNUPLOT were automated in PYTHON.

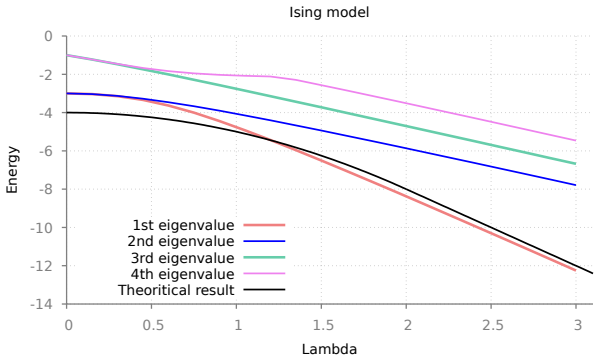
3 Results

Regarding the maximum number of particles tested, it was found to be $N = 10$. Figure 1 shows the first eigenvalues obtained for several number of spins. In particular, the code was run for a number of spins going from 2 to 10.

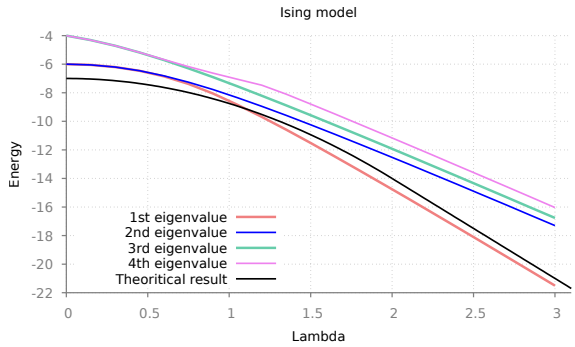


(a) N = 2.

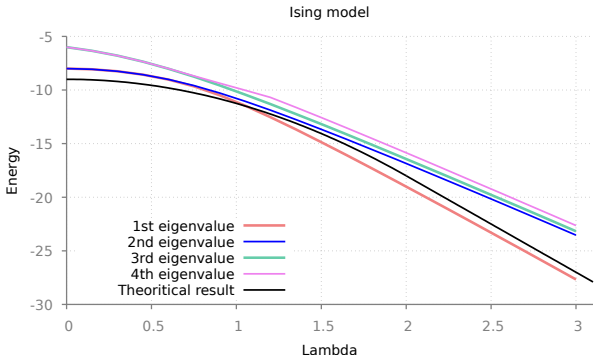
(b) N = 3.



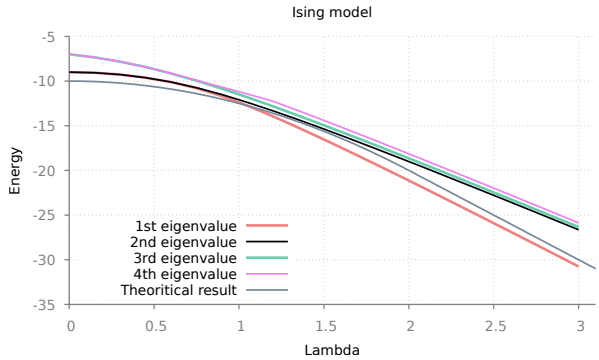
(c) N = 4.



(d) N = 7.



(e) N=9.



(f) N=10.

Figure 1. Comparison of first four eigenvalues obtained with several N

First of all, we notice that the spectrum of the system represent the energy levels accessible by the system itself. When the λ parameter is equal to 0 the system is described only by the second part of the Hamiltonian. As expected, a degeneration of the eigenvalues can be seen. For the case of $N = 2$ we can see that there are four configuration available: the less energetic one is the one with both spins in the direction of the magnetic field, the most energetic one is the one with both spins in the direction opposite of the field, and then there are two configurations with correspond

to the triplet and singlet state, with equal null energy.When λ increases we can see that the degeneration starts to break due to the the z-component spin interactions with an external magnetic field. Furthermore, a phase transition occur when passing from degenerate to not degenerate.

As expected, when increasing N the mean field solution resembles more to the theoretical result. Moreover, with high N the ground state becomes more distinct form the other energy levels which tend to come closer.

4 Conclusion

In conclusion, a N 1/2 - spin particle Ising model was successfully implemented. The Hamiltonian spectrum was found by implementing easily the LAPACK LIBRARY. Moreover, a quantum phase transition was observed by changing the interaction term λ. The main drawback of the code is that it only allows to compute up to 10 particles since the Hamiltonian matrix is of order $2^N \times 2^N$ and becomes unfeasible.