Information Theory and Computation
Exercise 9

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Theory

In this exercise we are gonna diagonalize the Quantum Ising model with the Hamiltonian:

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

As a basis for the one particle Hilbert space we chose the one diagonalizing σ^z:

$$\sigma^z |0\rangle = |0\rangle \tag{2}$$

$$\sigma^z |1\rangle = -|1\rangle \tag{3}$$

An $N-$particles wave function is defined by a family of $\{n_i\}n_i = 0, 1$ i.e.

$$|n_1\rangle |n_2\rangle \dots |n_M\rangle \tag{4}$$

We can observe that there is a one to one correspondence between a wavefunction and an integer number form 0 to $2^N - 1$; from the coefficients above we obtain the number by computing:

$$n_1 + n_2 \times 2 + n_3 \times 2^2 + \dots + n_N \times 2^{N-1} \tag{5}$$

In other words, we treat the sequence $n_N n_{N-1} \dots n_1$ as a binary number. Since we chose the diagonal basis the action of $\sum_{i=1}^{N} \sigma_i^z$ on a N particles state is trivial; instead $\sigma_i^x \sigma_{i+1}^x$ as as:

$$\sigma_i^x \sigma_{i+1}^x |n_1\rangle |n_2\rangle \dots |n_M\rangle = |n_1\rangle |n_2\rangle \dots |1 - n_i\rangle |1 - n_{i+1}\rangle \dots |n_M\rangle \tag{6}$$

i.e. flips the i-th and the $i+1$-th spin. Denoting $|m\rangle = |m_1 m_2 \dots m_N\rangle$ and $|n\rangle = |n_1 n_2 \dots n_N\rangle$ with m and n constructed as above said, the matrix element $\langle m| \sigma_i^x \sigma_{i+1}^x |n\rangle$ is non zero if and only if the numbers m and n, in binary, have the same digits apart from the i-th and $i+1$-th, where they must be opposite; one can express this property by the following predicate:

$$\langle m| \sigma_i^x \sigma_{i+1}^x |n\rangle \neq 0 \leftrightarrow \mathrm{XOR}(n, 3 \times 2^{i-1}) == m \tag{7}$$

The XOR operation is done logically, bit-by-bit. The above property can be used to compute the Hamiltonian matrix elements:

$$H_{m,n} = \langle m| H |n\rangle = \lambda\delta_{m,n} + \sum_{i=1}^{N-1} \delta_{m,\mathrm{XOR}(n,3\times 2^{i-1})} \tag{8}$$

The number $3\times 2^{i-1}$ is a *mask* number, useful to compare the bits of each index m and n: it is equal to the binary 11_2 shifted towards the left in order to force the i-th nd $i+1$-th bits to be opposite (an the others to be equal). Practically, given some m, look for all the n's that have non zero $\delta_{m,\mathrm{XOR}(n,3\times 2^{i-1})}$, for $i = 1 \dots N-1$.

Code Development

Essentially we need two function to build the Hamiltonian; the first one is the function computing the magnetization for a given state (i.e. the first part of the Hamiltonian); basically, for a state indexed by the number n, the magnetization is given by the number of zeros minus the number of ones in the binary representation:

```
function magnetization_integer(x, N)result(mgn)
        integer*4, intent(in) :: x,N
        integer*4 :: ii, mgn
        mgn = 0
        do ii=0,N-1
                if(BTEST(x, ii))then
                        mgn = mgn - 1
                else
                        mgn = mgn + 1
                end if
        end do
end function
```

The second function we need is the one that actually computes the Hamiltonian matrix elements:

```
function isingHamiltonian(N,lmbd)result(H)
        integer*4, intent(in) :: N
        real*8, intent(in) :: lmbd
        complex*16, dimension(:,:), allocatable :: H
        integer*4 :: sz,mm,nn,mask,kk
        sz = 2**N
        allocate(H(sz,sz))
        H = 0
        do mm=0,sz-1
                H(mm+1,mm+1)=lmbd*magnetization_integer(mm, N)
                mask = 3
```

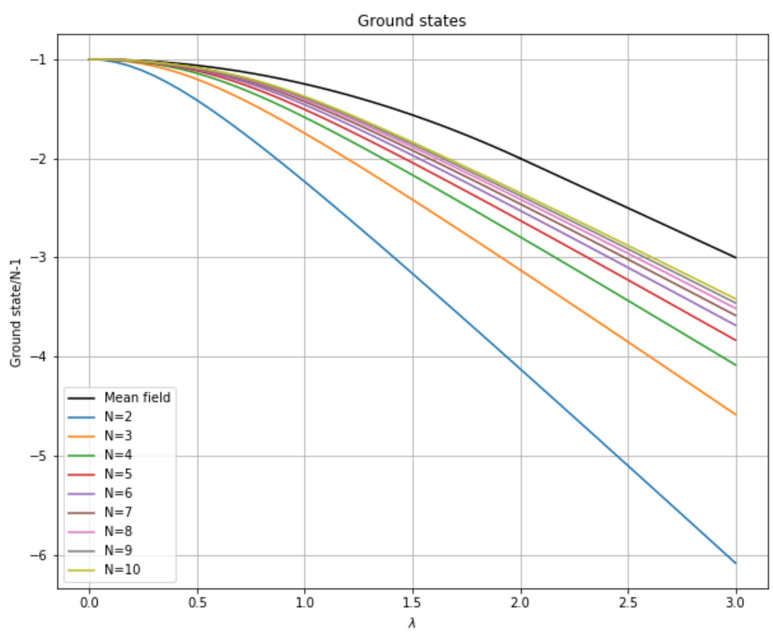
```
                do kk=1,N-1
                        nn = xor(mm,mask)
                        H(mm+1,nn+1)=1
                        H(nn+1,mm+1)=1
                        mask = mask*2
                end do
        end do
end function
```

The remaining part of the program had the job of diagonalizing the obtained matrix (via *zheev*) and saving the computed energies.

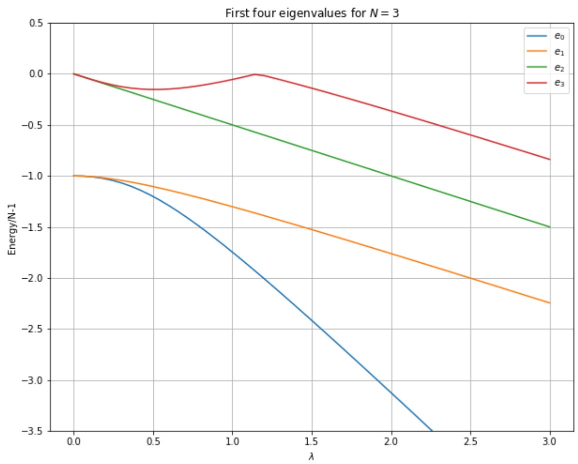
Results

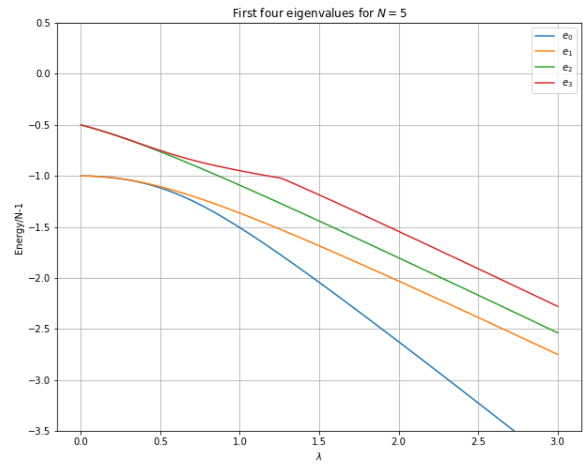
We run the code for a number of spins going from 2 to 10. Below we plot the ground state (divided by $N-1$) of each system and the mean field energy density which has the expression:

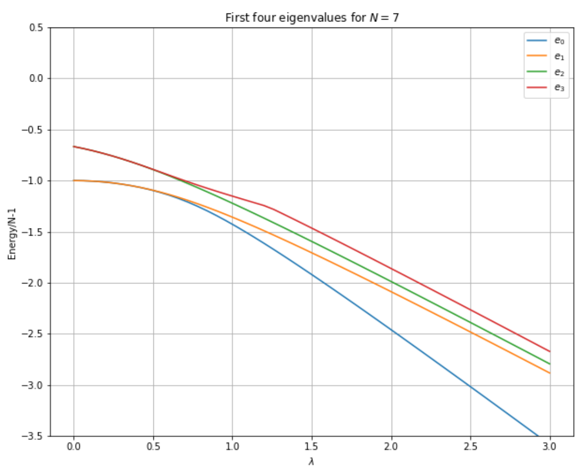
$$e_0(\lambda) = \begin{cases} -1 - \frac{\lambda^2}{4} & 0 < \lambda < 2 \\ -\lambda & \lambda > 2 \end{cases} \tag{9}$$

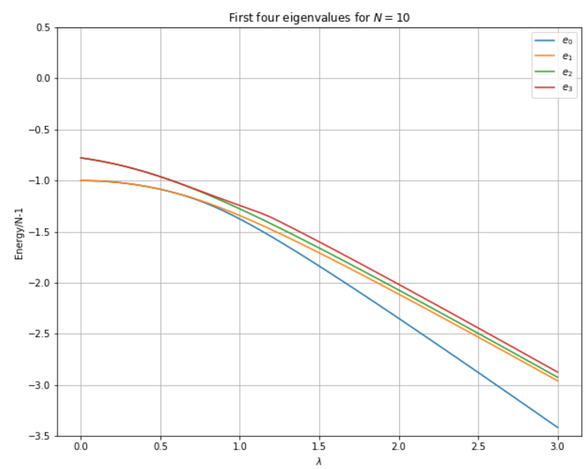


The computed ground states seem to look, as N highers, more similar to the mean field solution. Below, instead, we show, for some N's, the first four eigenvalues:









We can notice that as N highers the ground state is more and more distinct form the other energy levels which tend to come closer, especially at higher λ's. Another related interesting phenomenon that we observe is the degeneracy removal,due to leaving $\lambda = 0$.