Quantum information and computing: Report 9

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The Transverse filed Ising model was solved directly and the trend of the first excited states was studied when varying the number of interacting spins and the strength of the coupling

I. THEORY

The transverse field Ising model is a quantum version of the classical Ising model. It features a lattice with nearest neighbour interactions determined by the alignment or anti-alignment of spin projections along the z axis, as well as an external magnetic field perpendicular to the z axis which creates an energetic bias for one x-axis spin direction over the other.

An important feature of this setup is that, in a quantum sense, the spin projection along the x axis and the spin projection along the z axis are not commuting observable quantities. That is, they cannot both be observed simultaneously. This means classical statistical mechanics cannot describe this model, and a quantum treatment is needed.

In particular we can describe the 1D model with the Hamiltonian

$$H = \lambda \sum_{i}^{N} \sigma_z^{(i)} + \sum_{i}^{N-1} \sigma_x^{(i+1)} \sigma_x^{(i)}$$

Where λ is the coupling strength and $\sigma^{(i)}$'s are the Pauli matrices referring to the i-th spin in the chain. In particular this will be given by the application of the operator only on the relevant spin, while leaving the others unchanged and it is equivalent to the tensor product of the respective Pauli operator with identity operators for all the other spins.

II. CODE DEVELOPMENT

The code uses the same structure of previous exercises. In this case there 3 inputs: the number of spins and the coupling strength for the first and second term. In practice the constant of the second term has always been left equal to one during the exercise but it is present to have a more general code.

```
read(5,'(I10)',iostat=ierror) N
CALL FATAL( ierror > 0 ,      "main","Inputs
  are not integers" )

read (5,*) couple_1,couple_2
CALL FATAL(   N        <= 0 ,      "main","
  Number of q-bits" )
```

The Hamiltonian is then initialized using the input parameters in a dedicated module. The first and second term are computed separately and of the coupling constants have an absolute value smaller than the machine precision the respective piece of code is skipped to have a faster computation. The first term is computed first

```
IF (ABS(coupling_1) > EPSILON (coupling_1))
  THEN
    H = 0
    DO k=1,N
      swap = -1
      DO i = 1,2**N
          IF (MOD(i-1,INT(2**N/2**K)) == 0)
swap = -swap
          H(i,i) = H(i,i) + coupling_1*swap
      END DO
    END DO
  END IF
```

For the second term the matrix correspondent to the two Pauli matrices are computed independently and then a matrix multiplication is performed.

```
  IF(ABS(coupling_2) > EPSILON (coupling_2))
  THEN
    DO k=1,N-1
      int_1 = 0
      int_2 = 0
      DO m=1,INT(2**N/2**(k))
        DO i = 1,2**k
          IF (i > 2**(k-1) ) THEN
            int_1(i+(m-1)*2**k,i -2**(k-1) +(m
-1)*2**k) = int_1(i+(m-1)*2**k,i-2**(k-1)+(m
-1)*2**k) + 1
          ELSE
            int_1(i+(m-1)*2**k,i +2**(k-1) +(m
-1)*2**k) = int_1(i+(m-1)*2**k,i+2**(k-1)+(m
-1)*2**k) + 1
          END IF
        END DO
      END DO
      DO m=1,INT(2**N/2**(k+1))
        DO i = 1,2**(k+1)
          IF (i > 2**(k) ) THEN
            int_2(i+(m-1)*2**(k+1),i -2**(k)
+(m-1)*2**(k+1)) = int_2(i+(m-1)*2**(k+1),i
-2**(k)+(m-1)*2**(k+1)) + 1
          ELSE
            int_2(i+(m-1)*2**(k+1),i +2**(k)
+(m-1)*2**(k+1)) = int_2(i+(m-1)*2**(k+1),i
+2**(k)+(m-1)*2**(k+1)) + 1
          END IF
        END DO
      END DO

    !print *, int_2
!     print *, int_1
```

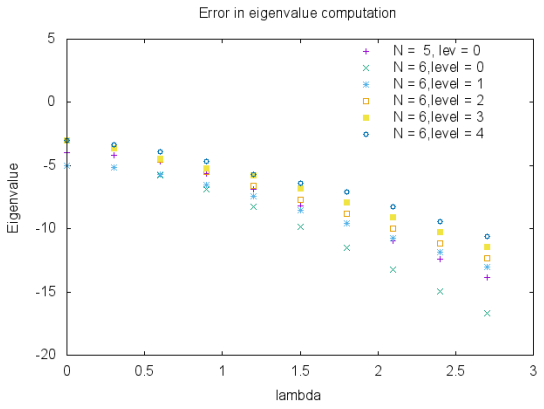

FIG. 1. First levels with 6 qubits

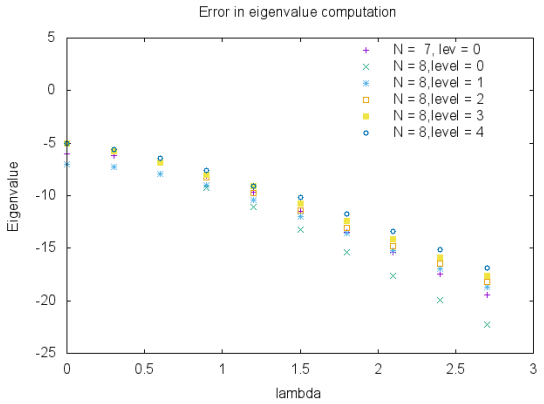

FIG. 2. First levels with 8 qubits

```
!     print*,H
      H = H + coupling_2*MATMUL(int_2,int_1)
      END DO
    END IF
```

Finally the diagonalization is performed using the zheev function in LAPACK

```
dim = 2**N
CALL zheev('N','U',dim,H,dim,egvals,WORK,LWORK
  ,RWORK,INFO)
CALL FATAL(INFO /= 0, "main", "Eigenvalues not
   found")
```

The script used also in previous versions of the code was modified to scan over N and λ as parameters.

III. RESULTS

The code has tested with N = 2 and N=3 to check its correctness. It has then been run with various values of N and the program crashes at N = 15 due to lack of memory. Using the Python script developed for previous exercises the code was tested for different values of N and λ and the plot of the first excited levels as a function of λ is shown in figures for different N in Fig.1-3. In every plot

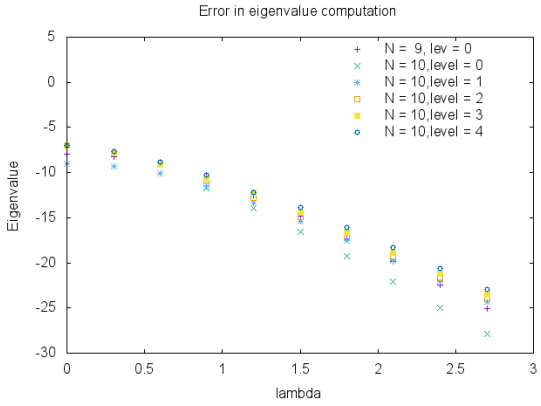

FIG. 3. First levels with 10 qubits

the ground state with N-1 qubits is also shown to compare the ground state energies. With $\lambda = 0$ the ground state is doubly degenerate with energy equal to -(N-1) and it corresponds to the case with all spins pointed in the same direction (recall that there are only N-1 terms of the type ${}^{(i+1)}\sigma^{(i)}$), the first excited state is also degenerate. This degeneracy is removed when lambda is greater than a critical value, where a quantum phase transition is present, and this critical value seems to increase with N. For a large enough N a convergence to the theoretical value of 1 is expected

IV. SELF-EVALUATION

The code has been modified to have the hamiltonian allocation in a different module in order to improve the flexibility. Furthermore the framework developed could be easily expanded to interactions with more than two bodies. An even more generalizable code could be implemented to work with any operator acting on only one spin, however this would not exploit the favorable properties of the Pauli matrices as the diagonal form of the σ_z.