Report: Week 7

Quantum Information and Computing (2021/22)
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Transverse-field Ising model (TFI)

We consider a quantum system formed by N spin-1/2 particles. The problem is given in an Hamiltonian represented by a $(2^N \times 2^N)$ matrix:

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

where we set $J = 1$. The notation simplifies the one of a **tensor product** that can be written as:

$$\sigma_i^z = \mathbb{1}_1 \otimes \cdots \mathbb{1}_{i-1} \otimes \sigma_i^z \otimes \mathbb{1}_{i+1} \otimes \cdots \mathbb{1}_N \tag{2}$$

$$\sigma_i^x \sigma_{i+1}^x = \mathbb{1}_1 \otimes \cdots \mathbb{1}_{i-1} \otimes \sigma_i^x \otimes \sigma_{i+1}^x \otimes \mathbb{1}_{i+2} \otimes \cdots \mathbb{1}_N. \tag{3}$$

λ is the **interaction strength parameter** and the σs are the **Pauli matrices** which do not commute:

$$[\sigma_i^j, \sigma_i^k] = 2i\varepsilon_{jk\ell}\, \sigma_i^\ell. \tag{4}$$

The system is built on a one-dimensional lattice with nearest neighbour interactions; an **external magnetic field** perpendicular to the x-axis causes an **energetic bias**.

The Hamiltonian presents a **spin-flip symmetry**.

The model can be exactly solved for all coupling constants: we observe 3 regimes.

Let $\Delta\mathcal{E}$ be the **energy gap** between the lowest excited state(s) and the ground state.

- **Ordered phase**. For $|\lambda| < 1$, the ground state breaks the spin-flip symmetry and is thus **two-fold degenerate**;

$$\Delta\mathcal{E} = 2|J|(1 - |\lambda|).$$

- **Disordered phase**. For $|\lambda| < 1$, the ground state preserves the spin-flip symmetry, and is **non-degenerate**;

$$\Delta\mathcal{E} = 2|J|(|\lambda| - 1).$$

- **Gapless phase**. When $|\lambda| = 1 \equiv \lambda_c$, the system undergoes a quantum phase transition.

Since we can only deal with a small number of spins N, the solutions are more precise in the **theormodynamic limit**, $N \to \infty$.

We compare the ground state with the **mean-field theory** predictions,

$$\mathcal{E}_0^{\mathrm{MF}}/N = \begin{cases} -1 - \lambda^2/4 & \lambda \in [-2, 2] \\ -|\lambda| & \text{otherwise.} \end{cases} \tag{5}$$

We investigate the spectrum for the first $K = 5$ eigenvalues, observing the behaviour of the system near the **quantum critical point** (QCP) at $\lambda = 1$.

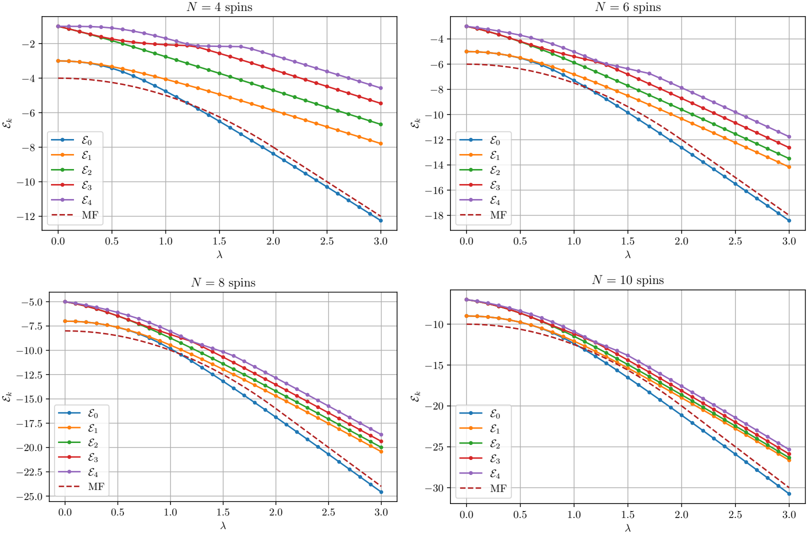
Listing 1: Implementation of the tensor product between two generic matrices.

```
allocate(M1_kp_M2(nr1*nr2,nc1*nc2))
! Initialise tensor product to zero
M1_kp_M2 = 0.0d0
forall ( ii = 1:nr1, jj = 1:nc1 ) &
M1_kp_M2(nr2*(ii-1)+1 : nr2*ii, nc2*(jj-1)+1 : nc2*jj)  =  M1(ii,jj)*M2
```

Listing 2: Implementation of the Ising Hamiltonian initialisation as in Eq. (2), (3).

```
allocate(ising(2**N,2**N))
! Initialise Hamiltonian to zero
ising = COMPLEX(0.0d0, 0.0d0)
! First term of the Ising Hamiltonian
do ii=1,N
    ising = ising + kronecker_product_c(                       &
                kronecker_product_c(identity_c(ii-1), s_z), &
                identity_c(N-ii)                            &
    )
end do
! Multiply by lambda
ising = COMPLEX(lambda,0.0d0) * ising
! Second term of the Ising Hamiltonian
do ii=1,N-1
    ising = ising - kronecker_product_c(                       &
                kronecker_product_c(                        &
                kronecker_product_c(identity_c(ii-1), s_x), &
                s_x), identity_c(N-ii-1)                    &
    )
end do
```

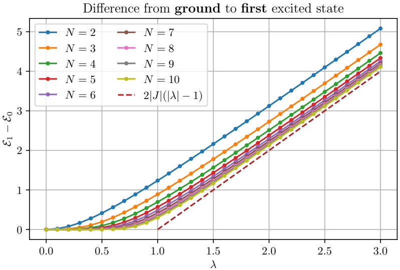
The time for the **initialisation** and **diagonalization** of the Hamiltonian is **exponential** in N. We thus consider $N < 10$ and run the code for $\lambda \in [0, 3]$.



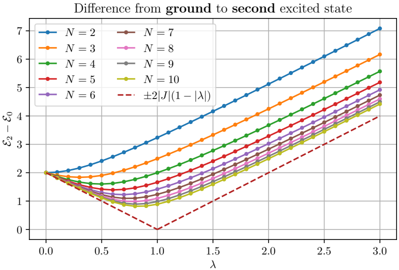
For a weak field ($\lambda \to 0$) the energy levels are degenerate as expected and the interaction term is dominating: all the spins are anti-aligned to minimise $\mathcal{E}$.

For a strong field ($\lambda \to \infty$) the external field is dominating and $\mathcal{E}_0$ approaches the MF solution. The QCP is pinched in $\lambda = 1$ for $N \to \infty$.

We plot here the energy gap between $\mathcal{E}_1 - \mathcal{E}_0$ (left) and $\mathcal{E}_2 - \mathcal{E}_0$ (right).



Below $\lambda = 1$ (QCP) the energy gap is 0: the ground state is two-fold degenerate.



The lowest excited state has energy $\mathcal{E}_2 > \mathcal{E}_0$ (non-vanishing for $N \to \infty$).