

Assignment 7

https://github.com/jchryssanthacopoulos/quantum_information/tree/main/assignment_7

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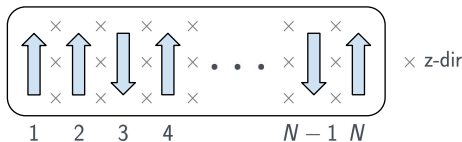


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- Quantum system composed of N spin-1/2 particles on one-dimensional lattice in presence of external magnetic field, with Hamiltonian

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

where σ_x and σ_z are Pauli matrices, and λ is interaction strength with magnetic field



- When $\lambda = 0$, ground state is when all neighbors have opposite spins, which can occur two different ways, with energy $-N + 1$. First excited state occurs when one spin is flipped, resulting in energy $-N + 3$
- When $\lambda \rightarrow \infty$, spins align to magnetic field and energies are $-\lambda N, -\lambda N + 2, \dots$

- Hamiltonian terms computed using **tensor product**, for example

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

- Example Hamiltonian for $N = 2$ system:

$$\hat{H} = \begin{pmatrix} 2 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & -2 \end{pmatrix}$$

```
function tensor_product(A, B) result(TP)
  implicit none

  integer ii, jj, kk, mm
  integer idx1, idx2
  integer N_A(2), N_B(2), N_TP(2)

  complex*16, dimension(:, :) :: A, B
  complex*16, dimension(:, :), allocatable :: TP

  N_A = shape(A)
  N_B = shape(B)
  N_TP = (/N_A(1) * N_B(1), N_A(2) * N_B(2)/)

  allocate(TP(N_TP(1), N_TP(2)))

  do ii = 1, N_A(1)
    do jj = 1, N_A(2)
      do kk = 1, N_B(1)
        do mm = 1, N_B(2)
          idx1 = (ii - 1) * N_B(1) + kk
          idx2 = (jj - 1) * N_B(2) + mm
          TP(idx1, idx2) = A(ii, jj) * B(kk, mm)
        end do
      end do
    end do
  end do
end function
```

```
function non_interacting_hamiltonian(N) result(H_0)
  implicit none

  integer N, dim
  integer ii
  complex*16 sigma_x(2, 2)
  complex*16, dimension(:, :), allocatable :: H_0, H_0_i

  complex*16, dimension(:, :), allocatable :: I1, I2, prod1

  sigma_x = (0d0, 0d0)
  sigma_x(1, 1) = (1d0, 0d0)
  sigma_x(2, 2) = (-1d0, 0d0)

  dim = size(sigma_x, 1) ** N

  allocate(H_0(dim, dim))

  H_0 = (0d0, 0d0)

  do ii = 1, N
    I1 = identity(ii - 1)
    I2 = identity(N - ii)
    prod1 = tensor_product(I1, sigma_x)

    H_0_i = tensor_product(prod1, I2)
    H_0 = H_0 + H_0_i

    deallocate(I1, I2, prod1, H_0_i)
  end do
end function
```

```
function interacting_hamiltonian(N) result(H_int)
  implicit none

  integer N, dim
  integer ii
  complex*16 sigma_x(2, 2)
  complex*16, dimension(:, :), allocatable :: H_int, H_int_i

  complex*16, dimension(:, :), allocatable :: I1, I2, prod1, prod2

  sigma_x = (0d0, 0d0)
  sigma_x(1, 1) = (1d0, 0d0)
  sigma_x(2, 2) = (-1d0, 0d0)

  dim = size(sigma_x, 1) ** N

  allocate(H_int(dim, dim))

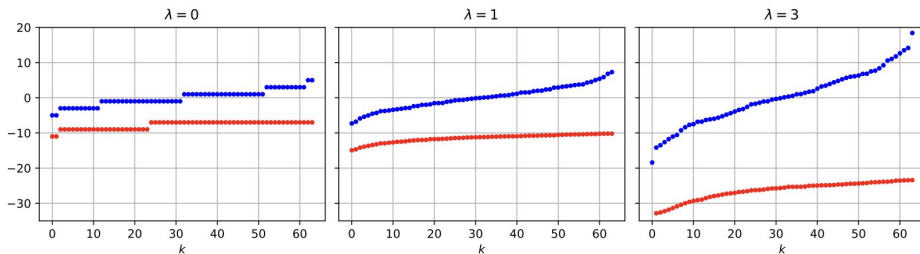
  H_int = (0d0, 0d0)

  do ii = 1, N - 1
    I1 = identity(ii - 1)
    I2 = identity(N - ii - 1)
    prod1 = tensor_product(I1, sigma_x)
    prod2 = tensor_product(prod1, sigma_x)

    H_int_i = tensor_product(prod2, I2)
    H_int = H_int + H_int_i

    deallocate(I1, I2, prod1, prod2, H_int_i)
  end do
end function
```

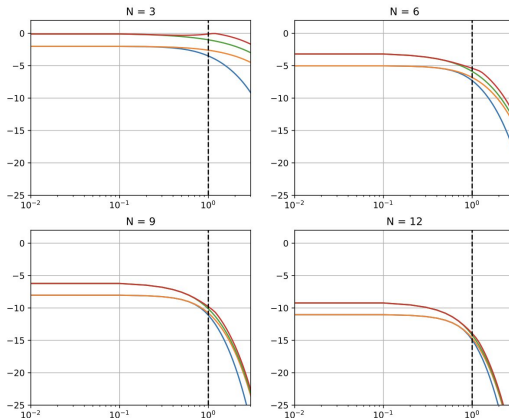
- When $\lambda = 0$, first two energies are degenerate with value $-N + 1$, as expected
- Each level separated by $\Delta E = 2$, and degeneracy increases with number of particles, as there are more combinations to produce same energy
- As λ increases, degeneracy is removed, but effect is less pronounced as N increases
- When λ is large, distinct mass gap forms for $N = 6$ particles



Energy Levels for Different λ and N



- First and second energy levels degenerate when λ is small
- Energy levels split when external magnetic field becomes strong enough
- Phase transition occurs when $\lambda \sim 1$, as expected



Energy Gap for Different λ and N



- Similar to last figure, energy gap between first and second levels becomes non-zero around $\lambda \sim 1$, but splitting shrinks with increasing N
- Difference between third and first levels non-zero even for small λ , making third level the first excited state, but again the gap shrinks with increasing N

