Assignment 7

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

Quantum Information and Computing
AA 2022–23

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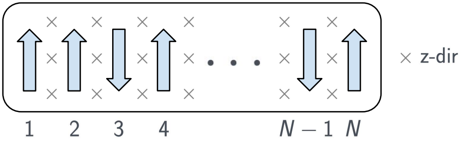
Quantum Ising Model

- 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 $\lambda \to \infty$, spins align to magnetic field and energies are $-\lambda N, -\lambda N + 2, \ldots$

Implementation

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

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

- Example Hamiltonian for $N = 2$ system with $\lambda = 1$:

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

```fortran
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
```

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

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

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

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

    dim = size(sigma_z, 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_z)

        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
```

```fortran
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, 2) = (1d0, 0d0)
    sigma_x(2, 1) = (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
```

- Diagonalization performed using `zheev`
- All eigenvalues for $N = 15$ computed in 16 hrs on Apple M1 Pro 32 GB

Energy Eigenvalues

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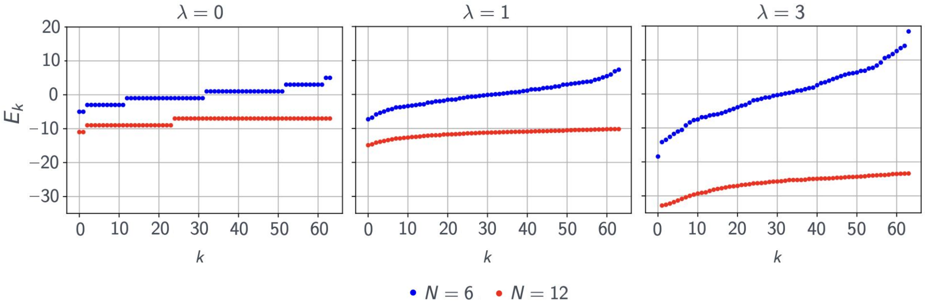
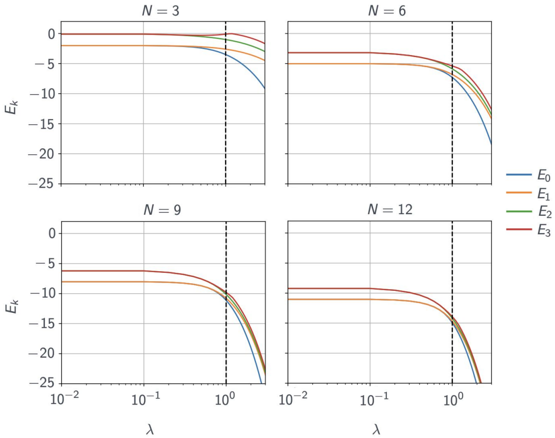
- When $\lambda = 0$, first two energies are degenerate with value $-N + 1$, as expected
- Each level separated by $\Delta E = 2$, and degeneracy increases with number of particles, as there are more combinations to produce same energy
- Energy decreases with N, because there are more spins
- As λ increases, 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