ASSIGNMENT 7

Physics of Data – Quantum Information and Computing

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THEORY (1)

- **Transverse field Ising model**

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

$$\sigma_i^z = \mathrm{I}_1 \otimes \cdots \otimes \mathrm{I}_{\mathrm{i}-1} \otimes \sigma_i^{\mathrm{z}} \otimes \mathrm{I}_{\mathrm{i}+1} \otimes \cdots \otimes \mathrm{I}_{\mathrm{N}}$$

$$\sigma_i^x \sigma_{i+1}^x = \mathrm{I}_1 \otimes \cdots \otimes \mathrm{I}_{\mathrm{i}-1} \otimes \sigma_i^{\mathrm{x}} \otimes \sigma_{i+1}^{\mathrm{x}} \otimes \mathrm{I}_{\mathrm{i}+2} \otimes \cdots \otimes \mathrm{I}_{\mathrm{N}}$$

- **Pauli matrices**
  - $\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
  - $\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

- **Total dimension**
  - N spin-½ particles on a 1D lattice (so each system has dimension 2).
  - Total dimension of the Hamiltonan is 2^N.

THEORY (2)

- **Quantum phase transition**
  - Quantum because $T = 0$, the control parameter is not the temperature.
  - Occurs at $\lambda = \lambda_C = 1$, the critical transverse field strength.
  - Transition between ferromagnetic (ordered) and paramagnetic (disordered) phases → ground state changes non-analytically at λ_C

- **Energy gap**
  - $\Delta E = E_1 - E_0$
  - $\Delta E \to 0$ when $\lambda \to \lambda_C$

- **Magnetization (order parameter)**
  - $M = \langle \sigma^z \rangle$
  - $M = -1$ for $\lambda < \lambda_C$
  - $M = 0$ for $\lambda > \lambda_C$

- **Von Neumann entropy**
  - $S = -Tr(\rho_A \log \rho_A)$
  - $S \neq 0$ for $\lambda < \lambda_C$
  - $S = 0$ for $\lambda > \lambda_C$

- **Two-point correlation**
  - $C = \langle \sigma_i^z \sigma_{i+1}^z \rangle$
  - $C = 0$ for $\lambda < \lambda_C$
  - $C = 1$ for $\lambda > \lambda_C$

CODE DEVELOPMENT (1)

```
def ising_hamiltonian(N, l):
  …

  for i in range(N):
    zterm = sp.kron(sp.identity(2**i, format='csr'), sp.kron(s_z, sp.identity(2**(N - i - 1), format='csr')))
    H_nonint += zterm

  for i in range(N - 1):
    xterm = sp.kron(sp.identity(2**i, format='csr'), sp.kron(s_x, sp.kron(s_x, sp.identity(2**(N - i - 2),
format='csr'))))
    H_int += xterm

  H = H_int + l * H_nonint
  return H
```

```
def diagonalize_ising(N_values, l_values, k):
  …

  for N in N_values:
    x = min(k, N - 1)

    for l in l_values:
      H = ising_hamiltonian(N, l)

      eigval, eigvec = sp.linalg.eigsh(H, k=x, which='SA')  # Compute the smallest `k` eigenvalues
      eigvec = eigvec.T

      for i in range(x):
        eigvec[i] /= np.linalg.norm(eigvec[i])

      …
```

CODE DEVELOPMENT (2)

```
def energy_gaps(N_values, l_values,
                eigenvalues):
  …
  n = 2 if no_deg is True else 1
  # Loop over the values of N
  for N in N_values:
    gaps = []
    # Loop over the first k levels
    for l in l_values:
      gap = (eigenvalues[(N, l)][n] -
             eigenvalues[(N, l)][0]) / N
      gaps.append(gap)
        …
```

```
def magnetization(ground_state, N):
  …
  M_z = sp.csr_matrix((2**N, 2**N), dtype=complex)

  for i in range(N):
    M_z_i = sp.kron(sp.identity(2**i, format='csr’),
            sp.kron(s_z, sp.identity(2**(N - i - 1), format='csr')))
    M_z += M_z_i

  M_z /= N

  M = ground_state.conj().transpose().dot(M_z.dot(ground_state))
  return M
```

```
def von_neumann_entropy(state_vector, N, D,
                        keep_indices):
  …
  # Compute the reduced density matrix and its
eigenvalues
  reduced_density_matrix = rdm(state_vector, N, D,
keep_indices)
  eigenvalues =
np.linalg.eigvalsh(reduced_density_matrix)

  # Compute the Von Neumann entropy
  entropy = -np.sum(non_zero_eigenvalues *
np.log(non_zero_eigenvalues))
  return entropy
```

```
def two_point_correlation(psi, N, i):

  …

  # Construct σ_z^i σ_z^i+1 operator
  operator = sp.kron(sp.identity(2**i, format='csr'),
sp.kron(s_z, sp.kron(s_z, sp.identity(2**(N - i - 2),
format='csr'))))

  # Compute the expectation value
  correlation = np.real(ground_state.conj().transpose()
                .dot(operator.dot(ground_state)))

  return correlation
```

RESULTS (1)

- **Implementation with normal matrices**

- $N_{\max} = 14$, so the Hamiltonian has size 2^{14} (for $N = 15$ we exceed the storage limit).

- For $N = 11$, we need around 33 Mb to store the Hamiltonian, for $N = 14$ we need around 1 Gb.

$$\begin{pmatrix} 20 & 0 & 0 & 3 \cdots & 0 \\ 0 & -16 & 1 & 0 \dots & \vdots \\ & \vdots & & & \vdots \\ & 0 & & & 20 \end{pmatrix}$$

- **Implementation with sparse matrices**

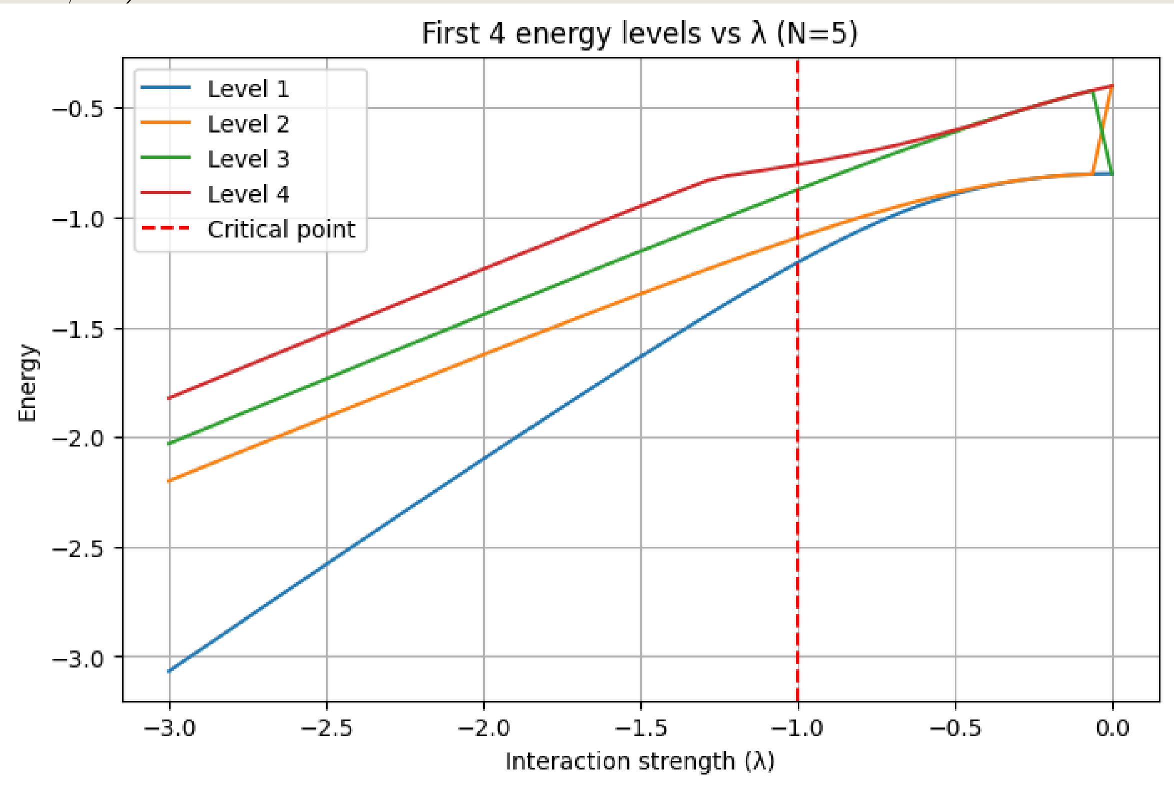
- $N_{\max} = 19$ (for higher N the kernel crashes).

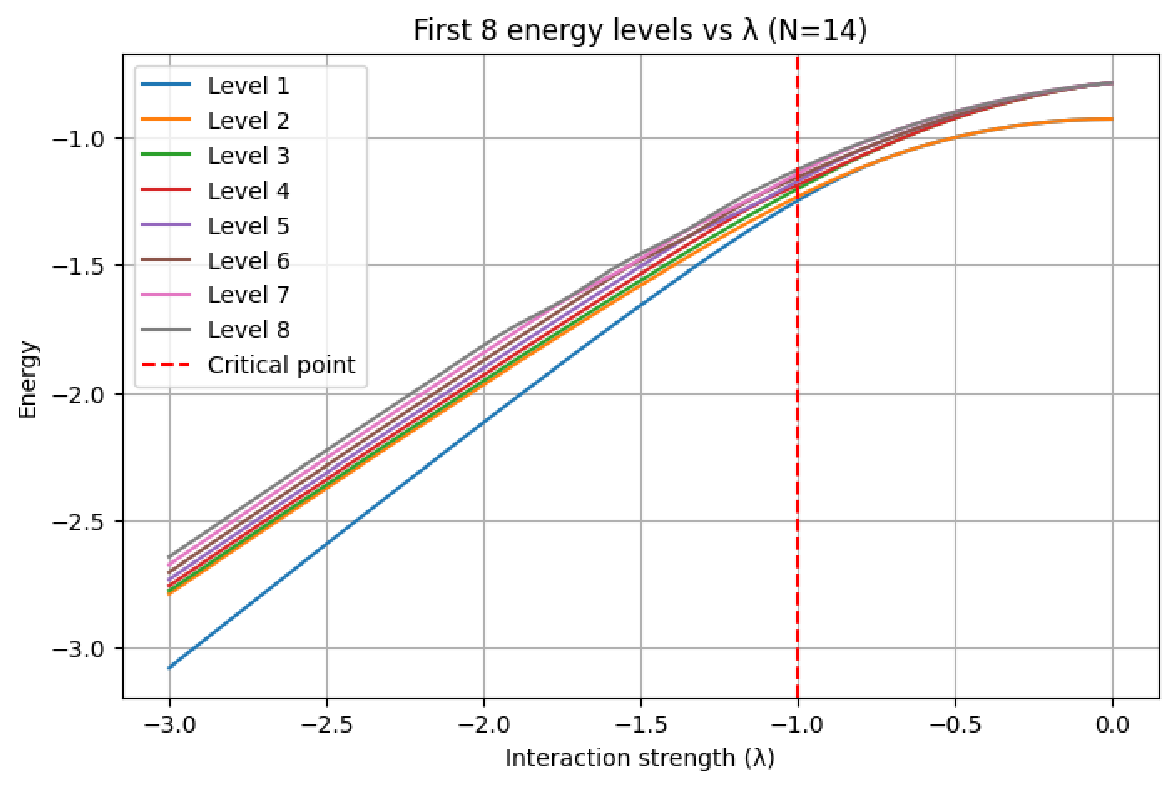
- For $N = 30$, we need around 8 Gb to store the Hamiltonian, even if sparse.

```
(0, 0) (-20+0j)
(0, 3) (1+0j)
(0, 6) (1+0j)
(0, 12) (1+0j)
(0, 24) (1+0j)
(0, 48) (1+0j)
(0, 96) (1+0j)
(0, 192) (1+0j)
(0, 384) (1+0j)
(0, 768) (1+0j)
(1, 1) (-16+0j)
(1, 2) (1+0j)
```

```
 :      :
(1022, 1022) (16+0j)
(1023, 255) (1+0j)
(1023, 639) (1+0j)
(1023, 831) (1+0j)
(1023, 927) (1+0j)
(1023, 975) (1+0j)
(1023, 999) (1+0j)
(1023, 1011) (1+0j)
(1023, 1017) (1+0j)
(1023, 1020) (1+0j)
(1023, 1023) (20+0j)
```

RESULTS (2)

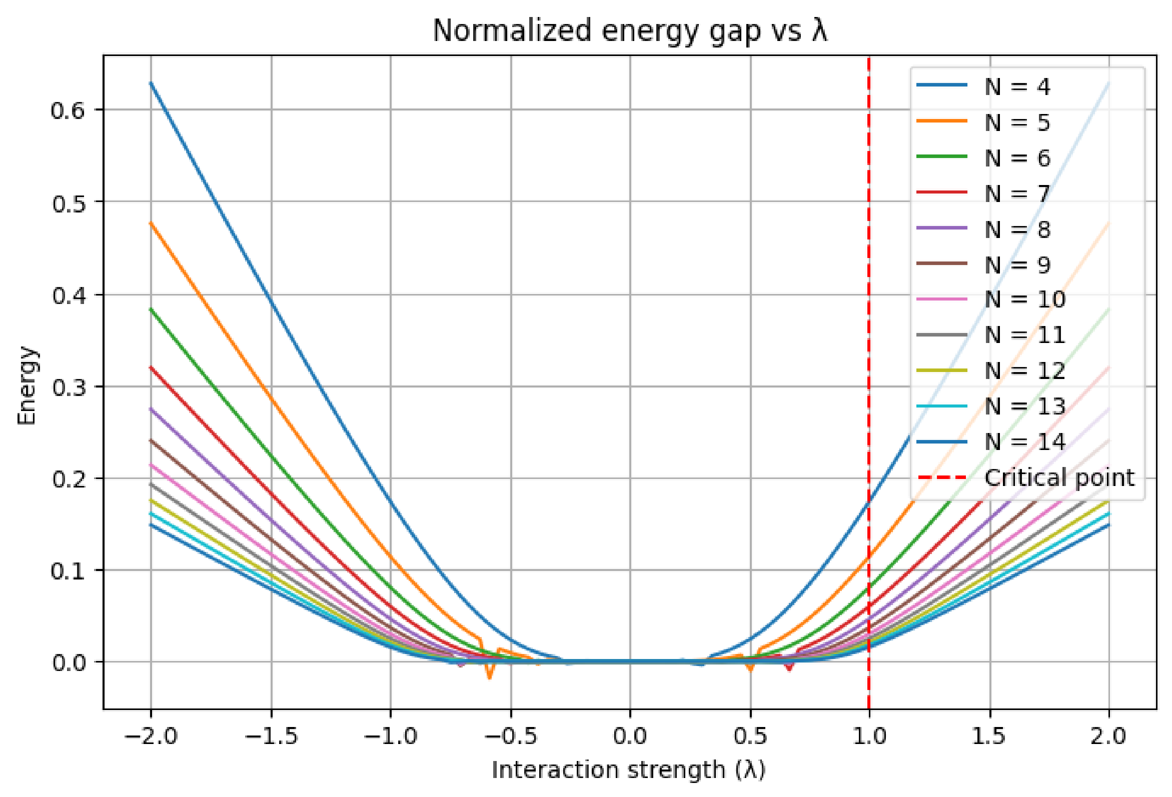


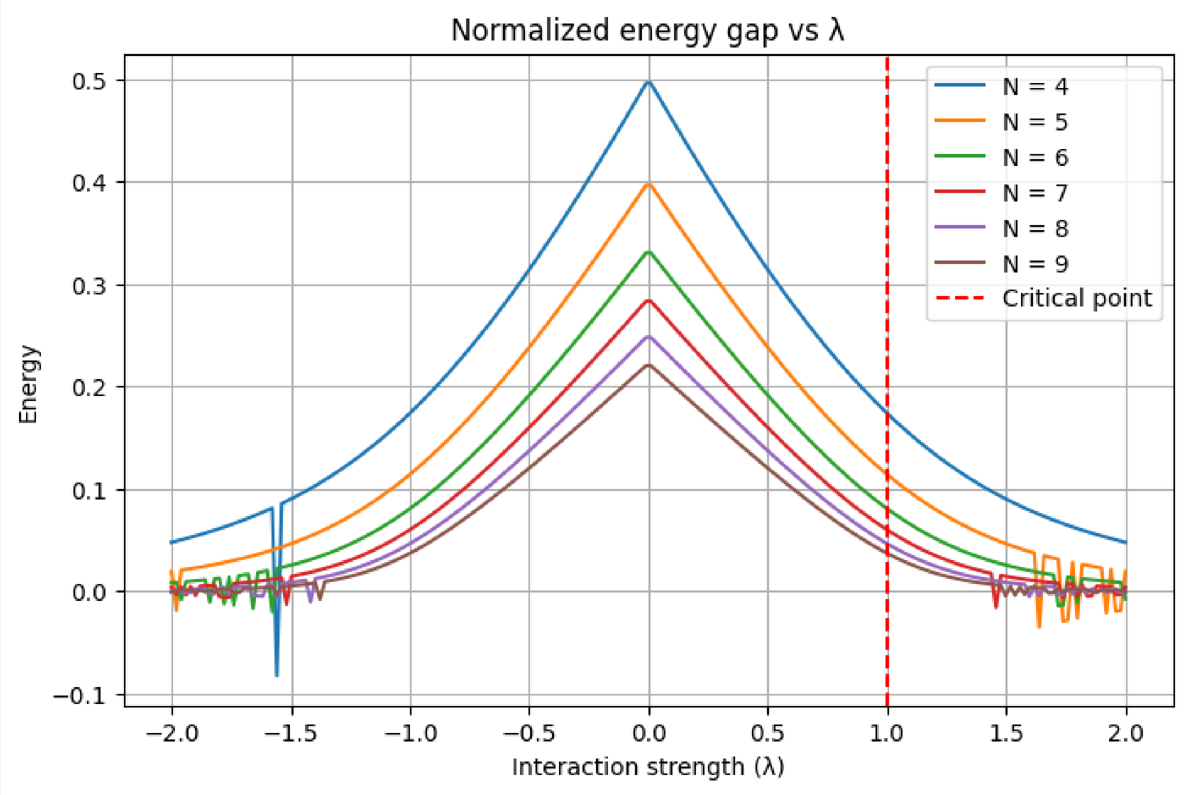


- Same GS behaviour
- Different behaviour of the excited states: for higher N we have a denser spectrum

- For $\lambda = 0$ we have degeneracy
- For $\lambda \to -\infty$ the degeneracy between the GS and the first excited state vanishes

PHASE TRANSITION (1)

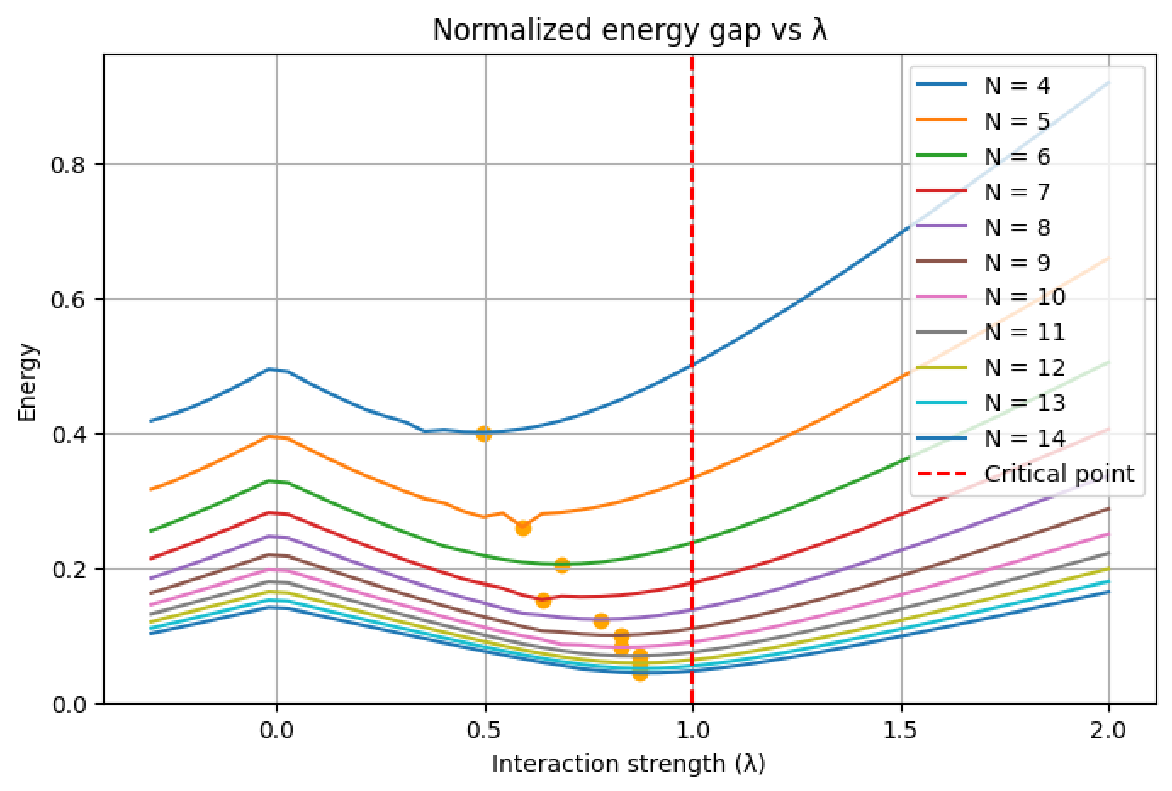


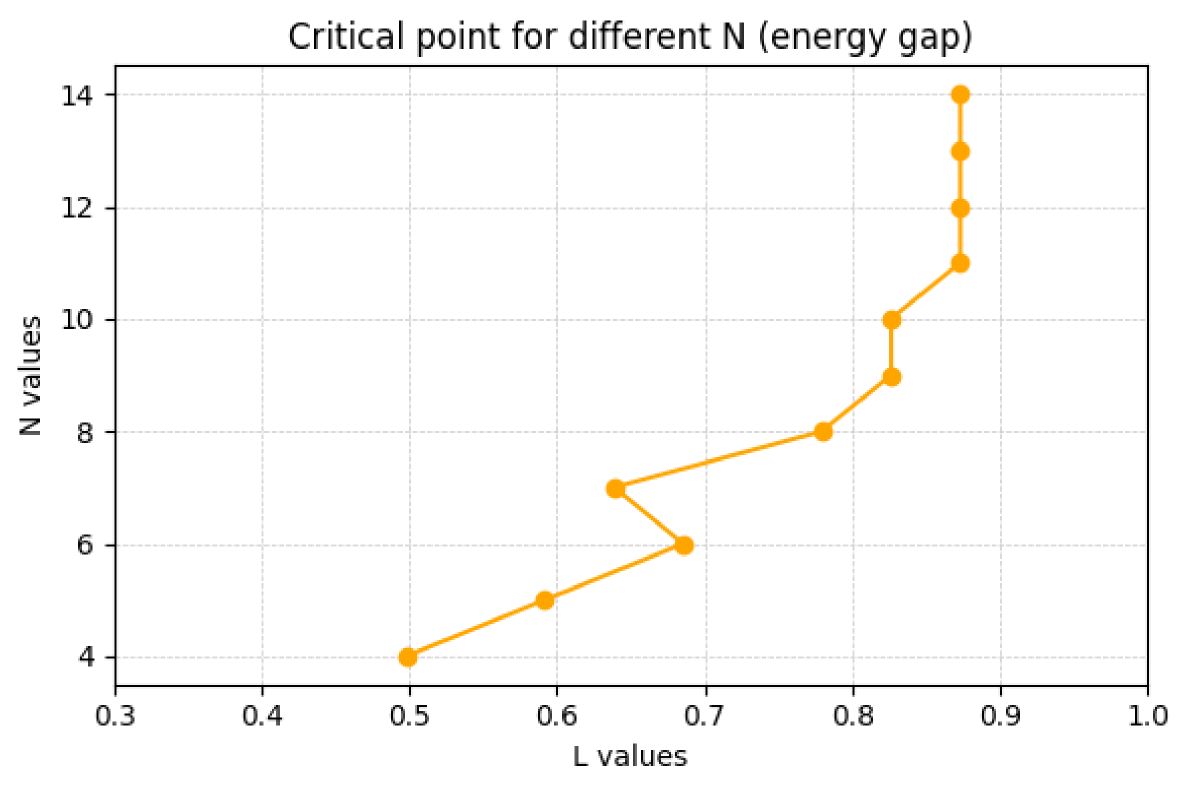


$$\hat{H} = \lambda \sum_{i=1}^{N} \sigma_i^z + \sum_{i=1}^{N-1} \sigma_i^x \sigma_{i+1}^x$$

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

PHASE TRANSITION (2)



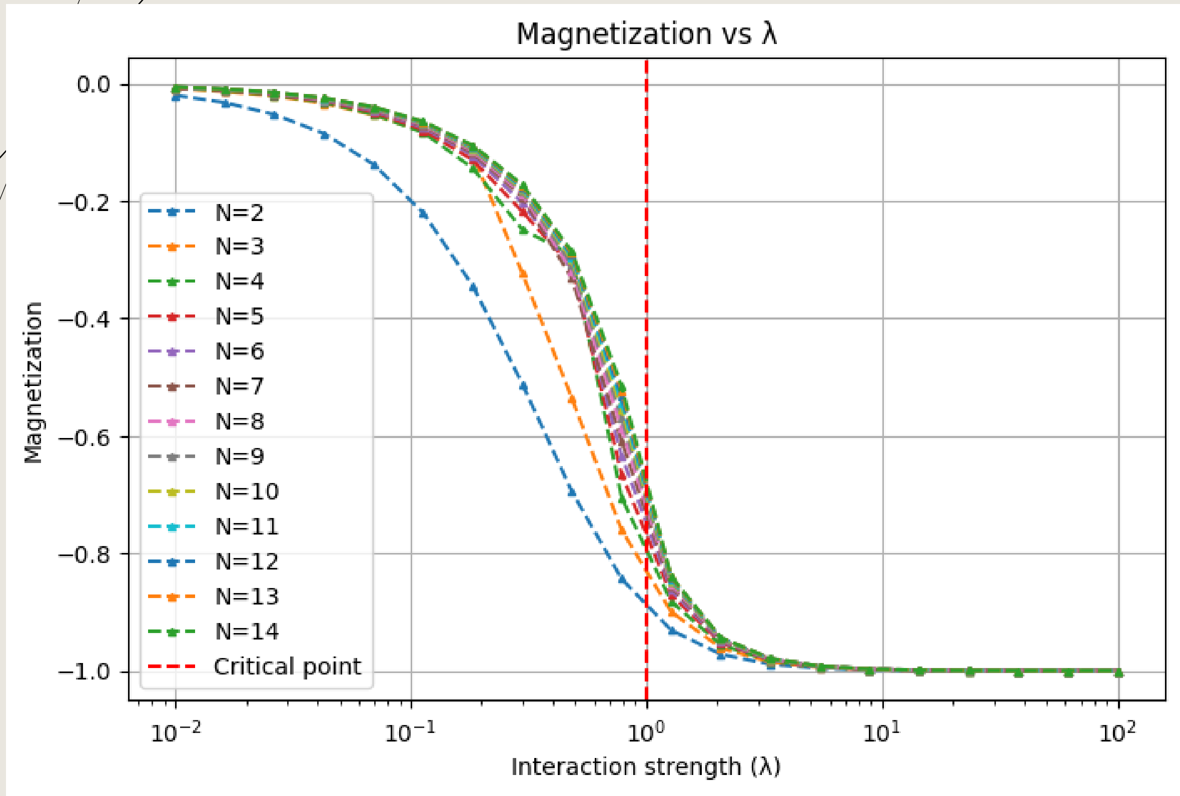


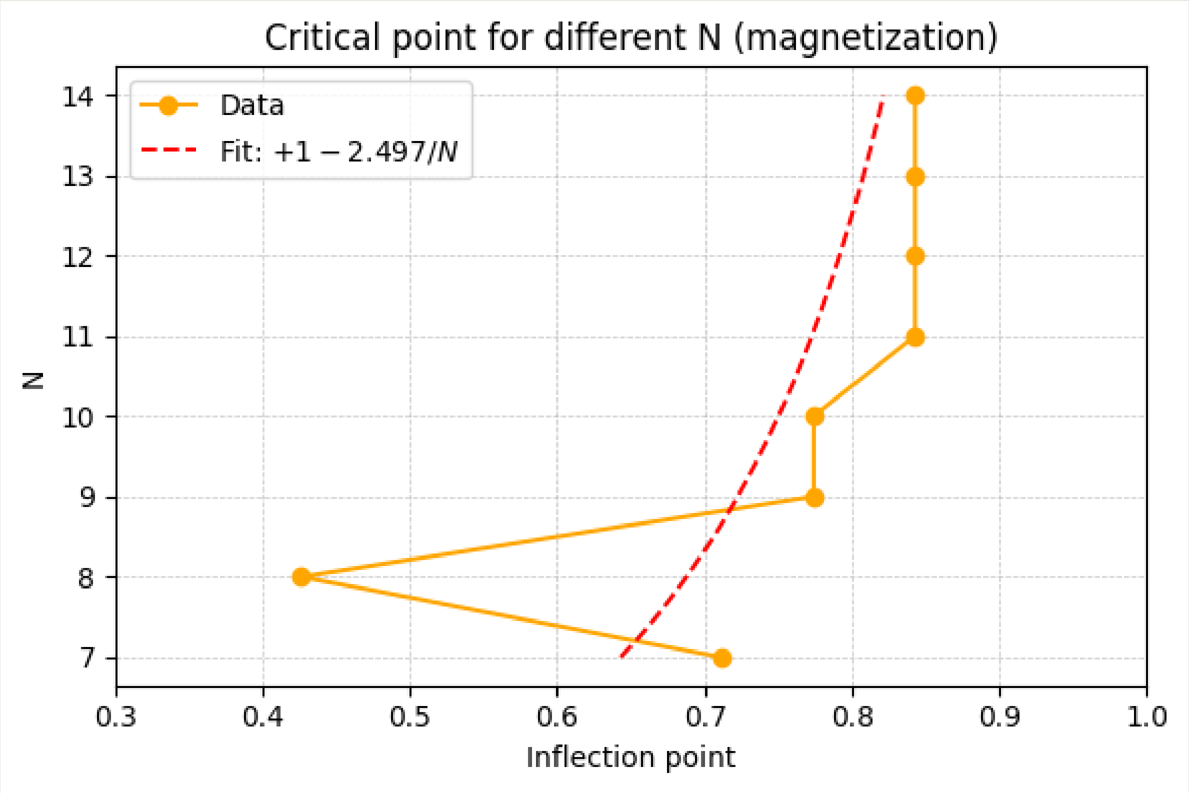
- ❑ Energy gap between GS and the second excited state (no degeneracy)
- ❑ Minimum value when $\lambda \to \lambda_c$

$$\lambda_c \to 1 \quad \text{for} \quad N \to +\infty$$

$$\Delta E \to 0 \quad \text{for} \quad N \to +\infty$$

PHASE TRANSITION (3)



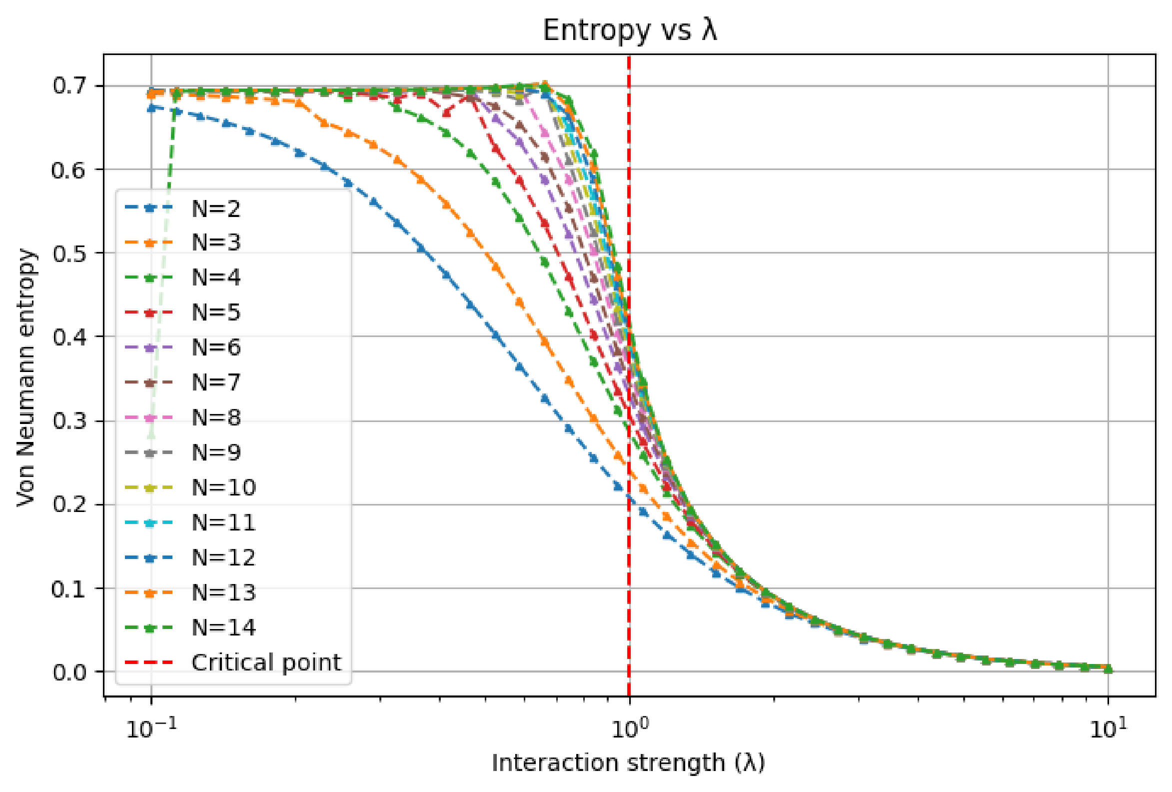


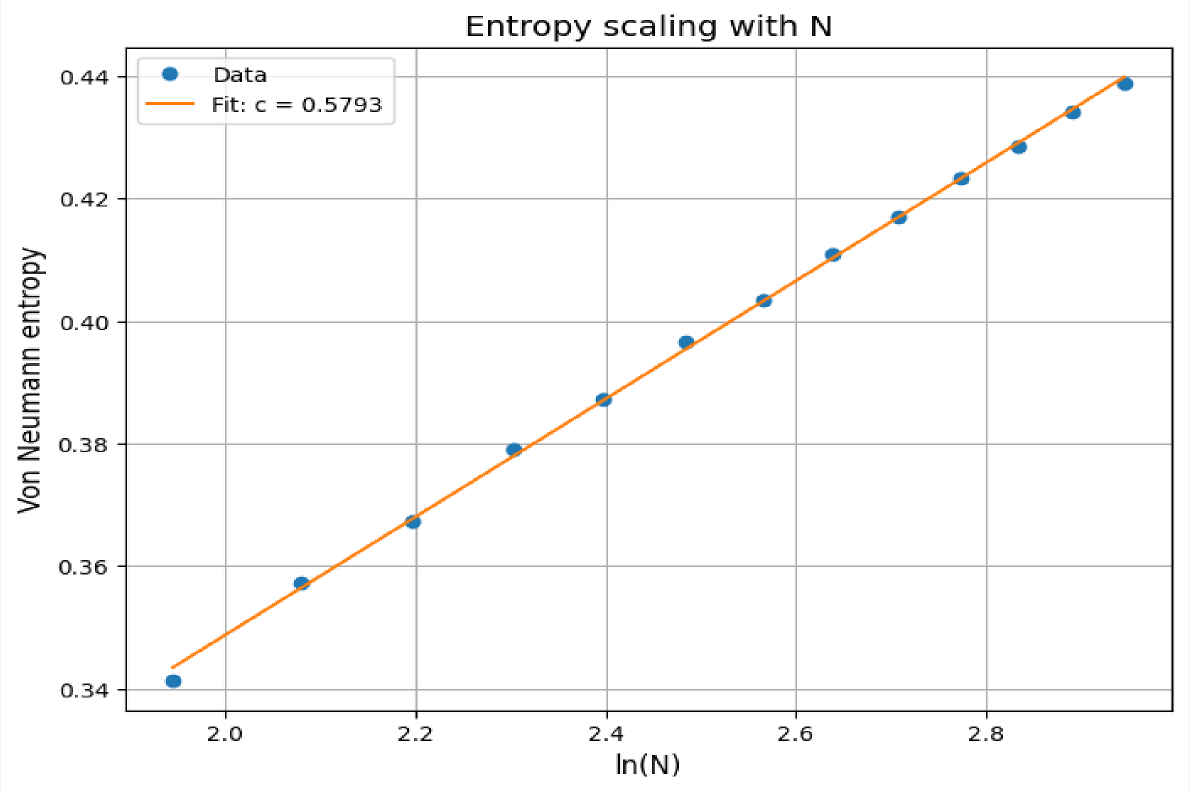
- ❑ $M = 0$ for small λ (disordered phase)
- ❑ $M = -1$ for high λ (ordered phase)

$$\lambda_c \rightarrow 1 \quad \text{for} \quad \mathrm{N} \rightarrow +\infty$$

$$f = 1 + \frac{a}{N} \qquad a = -2.50 \pm 0.07$$

PHASE TRANSITION (4)



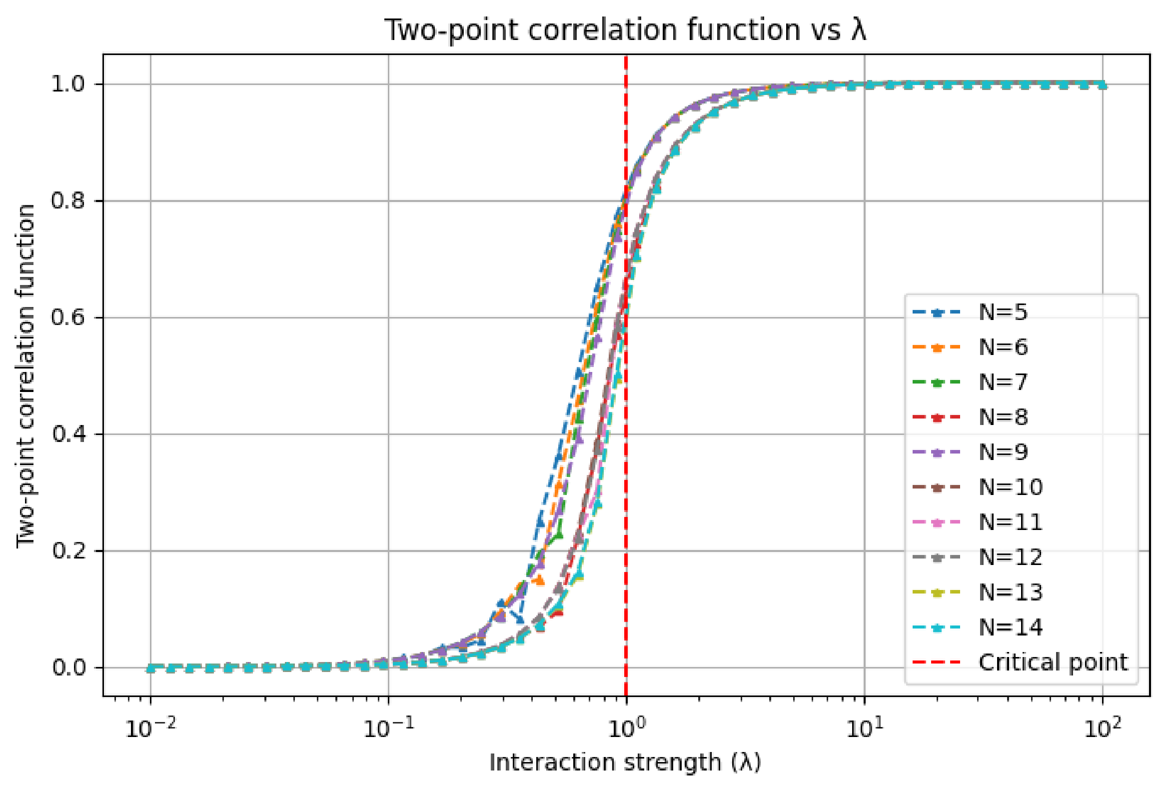


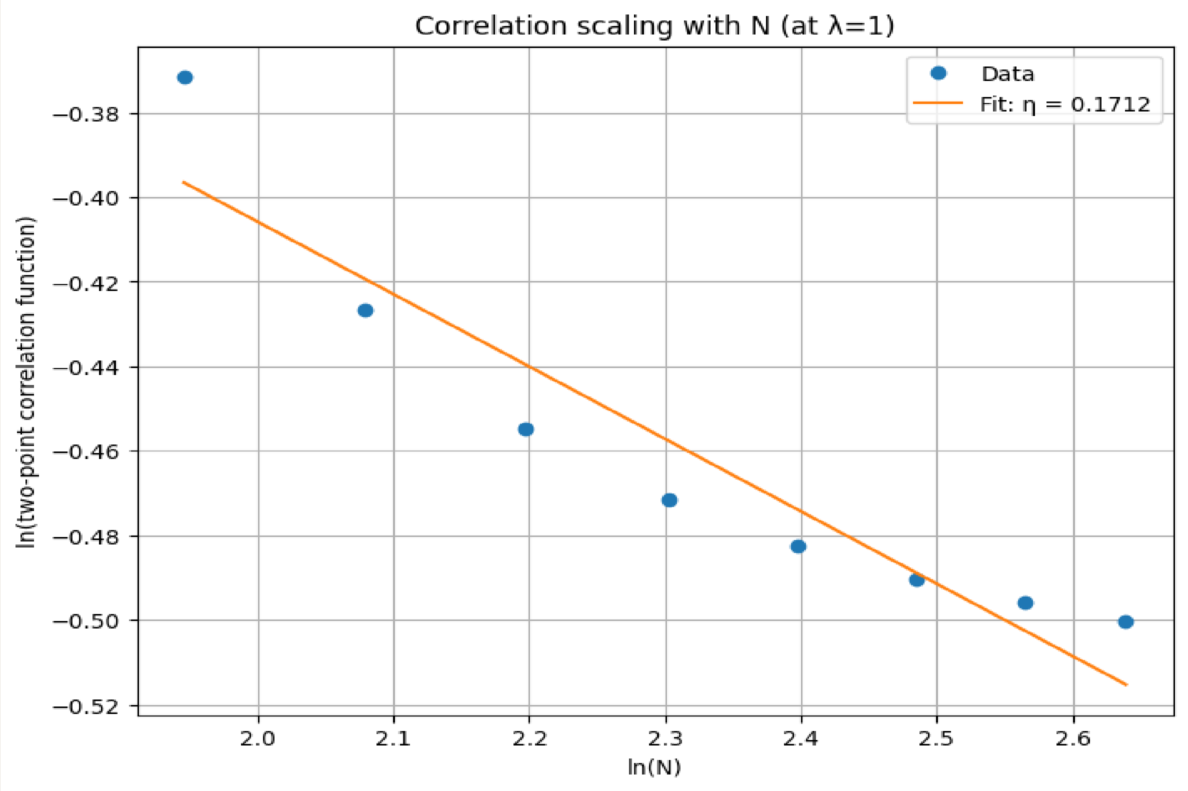
- ❑ $S = 0$ for high λ (ordered phase)
- ❑ $S \neq 0$ for small λ (disordered phase)

$$S = N^C + a \quad \rightarrow \ln S = C \ln N + const$$

$$\text{from the fit} \rightarrow C = 0.579 \pm 0.005$$

PHASE TRANSITION (5)





- ❑ $C = 0$ for small λ (disordered phase)
- ❑ $C = 1$ for high λ (ordered phase)

$$C = N^{\eta} + a \quad \rightarrow \ln C = \eta \ln N + const$$

- ❑ The fit doesn’t seem to be linear (exponential?)

CONCLUSIONS

- **Ising model:**
  - Usage of sparse matrix allows for a higher N, even though it is still low (max 19).
  - The spectrum presents degeneracy for $\lambda = 0$.

- **Phase transition:**
  - The energy gap between GS and the second excited state behaves as expected, reaching a minimum when $\lambda \to \lambda_C$.
  - The magnetization behaves as expected, highlighting the transition from ferromagnetic to para-magnetic.
  - The Von Neumann entropy shows high entanglement for $\lambda \to 0$. The central charge obtained from the fit (when $\lambda = 0$) is near the expected value (0.5).
  - The two-point correlation function behaves as expected; when $\lambda = 0$ the correlation changes with N, but not with a polynomial relation.