THE UNIVERSITY OF HONG KONG
DEPARTMENT OF PHYSICS

# Assignment 3

Course: *Quantum Many-Body Computation (PHYS8202)* – Prof.*Zi Yang Meng*
Tutor: *Mr. Min Long, Mr. Shibo Shan*
Due date: *26th November, 2025*

**Exact Diagonalization of the Spin-1 Heisenberg Chain**

We have solved the spin-1/2 Heisenberg chain in the class. Now, consider the spin-1 Heisenberg chain with periodic boundary conditions ($\vec{S}_N = \vec{S}_0$):

$$H = J\sum_{i=0}^{N-1} \vec{S}_i \cdot \vec{S}_{i+1} = J\sum_{i=0}^{N-1}\left[\frac{1}{2}\left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right) + S_i^z S_{i+1}^z\right]$$

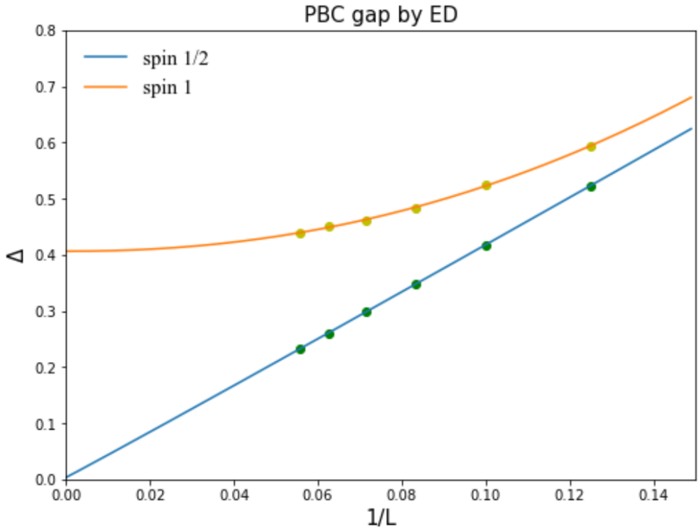
1. Choose the $S^z$ basis:
$$|S_0^z, S_1^z, \ldots, S_{N-1}^z\rangle,$$
where $S_i^z = 0, \pm 1$. Construct the spin-1 chain Hamiltonian matrix and obtain its eigen-energies.

2. Consider magnetization conservation:
$$m_z = \sum_i S_i^z, \quad [m_z, H] = 0$$
Sort the basis states according to their magnetization eigenvalue $m_z$, construct the corresponding block-diagonal Hamiltonian matrix, and find the eigenvalues of each block.

3. Next, take into account the translational symmetry of the system:
$$[T, H] = 0,$$
where
$$T|S_0^z, S_1^z, \ldots, S_{N-1}^z\rangle = |S_{N-1}^z, S_0^z, \ldots, S_{N-2}^z\rangle$$
Further decompose each $m_z$ block into smaller blocks corresponding to different momentum, and compute the eigenvalues of the smaller blocks. Plot the eigenvalues versus momentum for $m_z = 0, \pm 1$ blocks in three separate figures

4. Use the Lanczos algorithm to calculate the smaller blocks derived in problem 3, try to find the ground state and first excited state energies of the spin-1 Heisenberg chain for different system sizes $N$. Also determine the quantum number $m_z$ and $k$ for both ground state and first excited state. Plot the energy gap versus $1/N$, and perform an extrapolation to verify that in the thermodynamic limit

($N \to \infty$), the spin-1 Heisenberg chain is gapped. The example plot is shown below as the orange line.




From Prof.Han-Qing Wu of SYSU