EXACT VALUE OF THE GROUND STATE ENERGY
OF THE LINEAR ANTIFERROMAGNETIC HEISENBERG CHAIN
WITH NEAREST AND NEXT-NEAREST NEIGHBOUR INTERACTIONS

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It is shown that the ground state energy of the hamiltonian

$$H = \sum S_i \cdot S_{i+1} + \gamma \sum S_i \cdot S_{i+2}$$

for the linear antiferromagnetic Heisenberg chain with nearest and next-nearest neighbour interactions is equal to $-\frac{3}{2}$ if $\gamma = \frac{1}{2}$.

We consider the linear antiferromagnetic Heisenberg chain with nearest and next-nearest neighbour interactions with hamiltonian

$$H_N(\gamma) = \sum_{i=1}^{N-1} S_i \cdot S_{i+1} + \gamma \sum_{i=1}^{N-2} S_i \cdot S_{i+2},$$

where $N$ is the number of spins $\frac{1}{2}$ in the chain. Let the lowest eigenvalue of $H_N(\gamma)$ be $E_N(\gamma)$. We are interested in the energy per spin in the ground state in the limit of large $N$:

$$E(\gamma) = \lim_{N \to \infty} E_N(\gamma)/N.$$

$E(0)$ is known exactly [1,2]; it is equal to $1 - 4 \ln 2$ ($= -1.7726, ...$). For $\gamma \not= 0$ only approximations and upper and lower bounds for $E(\gamma)$ are known [3-8]. Majumdar and Ghosh [3,4] have found that for small finite chains ($N < 10$) with an even number of spins and periodic boundary conditions $E_N(\frac{1}{2})$ is equal to $-\frac{3}{2}N$. Moreover they showed that $-\frac{3}{2}N$ is an eigenvalue of $H_N(\frac{1}{2})$ for all even $N$. The same is true for open chains with $N$ even [5]. Thus $E(\frac{1}{2}) \leq -\frac{3}{2}$. The aim of this note is to show that $E(\frac{1}{2})$ is equal to $-\frac{3}{2}$ and that $E(\gamma)$ takes its maximal value at $\gamma = \frac{1}{2}$.

Divide the chain into $\frac{N}{2}$ cells of 2 spins. Let the state $|\psi\rangle$ of the chain be the direct product of the states, $2^{-1/2}(|+\rangle + |\rangle)$ for the cells. Then it is easy to verify that

$$H_N(\frac{1}{2}) |\psi\rangle = -\frac{3}{2}N |\psi\rangle,$$

and that

$$\langle\psi | H_N(\gamma) |\psi\rangle = -\frac{3}{2}N.$$

Therefore

$$E(\gamma) \leq -\frac{3}{2}.$$

This shows that $E(\gamma)$ takes its maximal value at $\gamma = \frac{1}{2}$ and that $E(\frac{1}{2}) = -\frac{3}{2}$; we calculate a lower bound for $E(\gamma)$.

The hamiltonian $H_N$ can be written as

$$H_N(\gamma) = \sum_{i=1}^{N-2} H_i(\gamma) + \frac{1}{2} S_1 \cdot S_2 + \frac{1}{2} S_{N-1} \cdot S_N,$$

where

$$H_i(\gamma) = \frac{1}{2} S_i \cdot S_{i+1} + \frac{1}{2} S_{i+1} \cdot S_{i+2} + \gamma S_i \cdot S_{i+2}.$$

Since, in general, the lowest eigenvalue of a sum of operators is not less than the sum of the lowest eigenvalues of these operators, the lowest eigenvalue of $H_N(\gamma)$ is not less than $(N-2)E_i(\gamma) - 3$ if $E_i(\gamma)$ is the lowest eigenvalue of $H_i(\gamma)$. $E_i(\gamma)$ can be calculated immediately; we find

$$E_i(\gamma) = \gamma - 2, \quad \text{if } \gamma \leq \frac{1}{2},$$

$$= -3\gamma, \quad \text{if } \gamma \geq \frac{1}{2}.$$  

Since $E_i(\frac{1}{2}) = -\frac{3}{2}$ it follows that $E_N(\frac{1}{2}) \geq -\frac{3}{2}N$. It
follows that \( E(\frac{1}{2}) \geq -\frac{3}{2} \) which proves that \( E(\frac{1}{2}) = -\frac{3}{2} \).

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References