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

P.M. van den BROEK
Department of Applied Physics, Twente University of Technology, Enschede, The Netherlands

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It is shown that the ground state energy of the hamiltonian $H = \Sigma S_i \cdot S_{i+1} + \gamma \Sigma S_i \cdot S_{i+2}$ 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

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

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:

$$E(\gamma) = \lim_{N\to\infty} E_N(\gamma)/N . \tag{2}$$

$E(0)$ is known exactly [1,2]; it is equal to $1 - 4 \ln 2$ ($= -1.7726, ...$). For $\gamma \neq 0$ only approximations and upper and lower bounds for $E(\gamma)$ are knwon [3–8]. Majumdar and Ghosh [3,4] have found that for small finite chains ($N \leqslant 10$) 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 $E(\frac{1}{2}) \leqslant -\frac{3}{2}$. 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 $\frac{1}{2}N$ 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

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

and that

$$\langle\psi|H_N(\gamma)|\psi\rangle = -\tfrac{3}{2}N . \tag{4}$$

Therefore

$$E(\gamma) \leqslant -\tfrac{3}{2} . \tag{5}$$

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

The hamiltonian H_N can be written as

$$H_N(\gamma) = \sum_{i=1}^{N-2} H_i(\gamma) + \tfrac{1}{2}S_1 \cdot S_2 + \tfrac{1}{2}S_{N-1} \cdot S_N , \tag{6}$$

where

$$H_i(\gamma) = \tfrac{1}{2}S_i \cdot S_{i+1} + \tfrac{1}{2}S_{i+1} \cdot S_{i+2} + \gamma S_i \cdot S_{i+2} . \tag{7}$$

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

$$\begin{aligned} E_i(\gamma) &= \gamma - 2 , \quad &\text{if } \gamma \leqslant \tfrac{1}{2} , \\ &= -3\gamma , \quad &\text{if } \gamma \geqslant \tfrac{1}{2} . \end{aligned} \tag{8}$$

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

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