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Abstract. The ground state of the one-dimensional antiferromagnetic model, with the Hamiltonian

$$H = \tfrac{1}{2}J \sum_{i=1}^{N} \boldsymbol{\sigma}_i.\boldsymbol{\sigma}_{i+1} + \tfrac{1}{4}J \sum_{i=1}^{N} \boldsymbol{\sigma}_i.\boldsymbol{\sigma}_{i+2}$$

($J > 0$, N even, $N + 1 \equiv 1$, $N + 2 \equiv 2$) can be given explicitly in terms of spin eigenfunctions. Various properties of the ground state are studied. An approximate determination of the low-lying excited states shows the usual linear frequency–wave-vector relationship.

1. Introduction

There are not many antiferromagnetic models for which the properties of the eigenstates are well known. For the linear chain of spin-$\frac{1}{2}$ particles with the Hamiltonian ($J > 0$)

$$H_0 = \tfrac{1}{2}J \sum_{i=1}^{N} \boldsymbol{\sigma}_i.\boldsymbol{\sigma}_{i+1} \tag{1.1}$$

the ground state energy is well known, and the structure of the ground state, as proved by Yang and Yang (1966a), is given by the Bethe *ansatz*. The form of the wave function is fairly complicated. It is known that the antiferromagnetic ground state of (1.1) has total spin $S = 0$ for even N (Lieb and Mattis 1962), but this feature is not apparent in the Bethe result. Several other antiferromagnetic models have been explicitly solved (Lieb *et al.* 1961, Katsura 1962) by transforming the spin problem into one of fermions, and then investigating the properties of these particles. To get a clearer understanding of the antiferromagnetic ground state, it is worth while to discuss a model for which the ground-state wave function can be simply written down in terms of α and β where α and β are the usual up and down spin eigenfunctions respectively. Unfortunately the model we are describing is one-dimensional, so many interesting and pertinent questions about long-range order cannot be answered. Also only an approximate determination of the low-lying excited states can be given.

2. Ground state

Consider the Hamiltonian of a chain of N spin-$\frac{1}{2}$ particles (N even, $N + 1 \equiv 1, N + 2 \equiv 2$)

$$H = \tfrac{1}{2}J \sum_{i=1}^{N} \boldsymbol{\sigma}_i.\boldsymbol{\sigma}_{i+1} + \tfrac{1}{4}J \sum_{i=1}^{N} \boldsymbol{\sigma}_i.\boldsymbol{\sigma}_{i+2}. \tag{2.1}$$

The second neighbours interact with a strength exactly half that of the nearest neighbours. Such a Hamiltonian with second-neighbour interaction present in varying fractional strength relative to that of the first neighbours has been studied in detail by Majumdar and Ghosh (1969). From their work the following result for (2.1) follows. Introduce the notation

$$[l\,m] = \alpha(l)\,\beta(m) - \beta(l)\,\alpha(m). \tag{2.2}$$

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Construct the functions

$$\phi_1 = [1\,2]\,[3\,4]\ldots[N-3\,N-2]\,[N-1\,N] \tag{2.3}$$

$$\phi_2 = [2\,3]\,[4\,5]\ldots[N-2\,N-1]\,[N\,1]. \tag{2.4}$$

Then by direct calculation

$$H\phi_1 = \tfrac{3}{4}JN\phi_1, \quad H\phi_2 = -\tfrac{3}{4}JN\phi_2. \tag{2.5}$$

A study of short chains provides convincing evidence that $-\frac{3}{4}NJ$ is indeed the ground-state energy.† Of course, any linear combination of ϕ_1 and ϕ_2 will belong to the same eigenvalue.

The ground-state wave function, however, must also diagonalize the translation operator simultaneously with the Hamiltonian. Let T be the operator which translates the chain by one unit distance. This is equivalent to the cyclic permutation

$$\begin{pmatrix} 1 & 2 & 3 & \ldots & N-1 & N \\ 2 & 3 & 4 & \ldots & N & 1 \end{pmatrix}.$$

Notice that

$$T\phi_1 = \phi_2, \quad T\phi_2 = \phi_1. \tag{2.6}$$

Hence the lowest energy state of the chain can be described either by the function Ψ_0^+ such that

$$\Psi_0^+ = \phi_1 + \phi_2, \quad T\Psi_0^+ = \Psi_0^+, \quad H\Psi_0^+ = -\tfrac{3}{4}NJ\Psi_0^+ \tag{2.7}$$

or by the function

$$\Psi_0^- = \phi_1 - \phi_2, \quad T\Psi_0^- = -\Psi_0^-, \quad H\Psi_0^- = -\tfrac{3}{4}NJ\Psi_0^-. \tag{2.8}$$

Since the functions ϕ_1 and ϕ_2 are built out of products of singlet combinations, the total spin must be zero, and of course the total $S_z = \frac{1}{2}\Sigma_i\sigma_i^z = 0$. Each spin is coupled in a singlet pair to its neighbour. The wave function is quite different from the alternating up and down spins often associated with the description of antiferromagnets; that such a picture is grossly inadequate for a Hamiltonian like (1.1) was noted by Marshall (1955).

One can now calculate the various correlation functions in the ground state. By straightforward calculation one can show that in the limit $N \to \infty$,

$$\langle\sigma_1^z\sigma_2^z\rangle_+ = \frac{\langle\Psi_0^+|\sigma_1^z\sigma_2^z|\Psi_0^+\rangle}{\langle\Psi_0^+|\Psi_0^+\rangle} = -\tfrac{1}{2} \tag{2.9}$$

$$\langle\sigma_1^z\sigma_3^z\rangle_+ = \langle\sigma_1^z\sigma_4^z\rangle_+ = \ldots = 0. \tag{2.10}$$

Also

$$\langle\sigma_i^z\sigma_j^z\rangle_- = \frac{\langle\Psi_0^-|\sigma_i^z\sigma_j^z|\Psi_0^-\rangle}{\langle\Psi_0^-|\Psi_0^-\rangle}$$

and

$$\langle\sigma_1^z\sigma_2^z\rangle_- = -\tfrac{1}{2}, \quad \langle\sigma_1^z\sigma_3^z\rangle_- = \langle\sigma_1^z\sigma_4^z\rangle_- = \ldots = 0. \tag{2.11}$$

Clearly the ground state has only short-range order and no long-range order. It is true that $\langle\sigma_1^z\sigma_N^z\rangle_+ = -\frac{1}{2}$ is finite, but this is a result of periodic boundary conditions. $\langle\sigma_1^z\sigma_{N-1}^z\rangle_+$ vanishes again. In other words the correlation falls off in either direction from any particular spin. The sign of the short-range order indicates that on the average an up spin is flanked by down spins.

† Dr J. Pasupathy has proved (private communication) that the ground state energy $E_0 \geqslant -\frac{3}{4}NJ$ for arbitrary N in (21).

Thouless (1967) studied a parameter

$$R_{ij} = \tfrac{1}{2}\langle(\sigma_i^x\sigma_j^x + \sigma_i^y\sigma_j^y)\rangle \tag{2.12}$$

to characterize the antiferromagnetic state. This gives zero when the two spins i and j are parallel but exchanges the spins when one is up and the other down. For the antiferromagnetic wave function considered by Marshall (1955) for the Heisenberg Hamiltonian R_{ij} is expected to have appreciable expectation value even when i and j are well separated. In our case we find that in the limit $N \to \infty$

$$R_{12} = -\tfrac{1}{2}, \qquad R_{13} = R_{14} = \ldots = 0. \tag{2.13}$$

The Thouless parameter is closely related to the off-diagonal long-range order discussed by C. N. Yang (Yang 1962, Yang and Yang 1966b). This involves the calculation of averages $\langle\sigma_i^+\sigma_j^-\rangle$ where $\sigma^\pm = \sigma^x \pm i\sigma^y$. We get, in the limit $N \to \infty$,

$$\langle\sigma_1^+\sigma_2^-\rangle_\pm = -1, \qquad \langle\sigma_1^+\sigma_3^-\rangle_\pm = \langle\sigma_1^+\sigma_4^-\rangle_\pm = \ldots = 0. \tag{2.14}$$

The correlation falls off as the separation increases. Since the model is one dimensional the absence of long-range order is not surprising, and the model tells us nothing about the corresponding quantities in higher dimensions.

3. Low-lying excited states

The determination of the excited states of (2.1) turns out to be difficult. One can check that the standard antiferromagnetic spin-wave approximation (Anderson 1952) breaks down and the spin waves do not have real frequency. The starting ground state in this approach is a poor representation of the ground states (2·7) and (2.8). An approximate determination of the low-lying excited states is possible, however, by the linearized equation of motion technique.

One may guess that the lowest excitations will be states with total spin $S = 1$. This is true of the short chain data of Majumdar and Ghosh (1969). For the standard linear chain (1.1), des Cloizeaux and Pearson (1962) made the same guess and obtained the exact dispersion law for these states by utilizing the Bethe *ansatz*.

The spin-1 states can be produced by breaking one or more singlet pairs in ϕ_1 and ϕ_2. Three operators which break one pair and produce a state of spin $S = 1$ are clearly $\sigma_i^\pm$ and σ_i^z for a particular i. One notices, for instance, that $\sigma_i^+\phi_1$ for various i will be $\frac{1}{2}N$ states of spin 1, in each of which exactly one ground state singlet pair has been broken. The states with one ground pair broken do not span the complete space of excited states of spin 1. Take the commutator

$$[\sigma_i^+, H] = J(\sigma_{i+1}^+ + \sigma_{i-1}^+)\sigma_i^z - J\sigma_i^+(\sigma_{i+1}^z + \sigma_{i-1}^z) + \tfrac{1}{2}J(\sigma_{i+2}^+ + \sigma_{i-2}^+)\sigma_i^z - \tfrac{1}{2}J\sigma_i^+(\sigma_{i+2}^z + \sigma_{i-2}^z). \tag{3.1}$$

Consider both sides of (3.1) operating on ϕ_1. Some terms on the right side clearly break up two pairs. Unlike the ferromagnetic case, where the fully aligned state is an eigenfunction of the individual σ_i^z, the equation does not linearize. An attempt to replace σ_i^z by its expectation value is meaningless, because this expectation value in the ground state is easily checked to be zero.

Intuitively one feels that the states with one ground singlet pair broken will form the dominant part of the wave function of the very low-lying states. So we try to get a linear equation for $\sigma^\pm$ and σ^z. One knows that

$$(\sigma_l^z)^2 = 1, \qquad \sigma_l^+\sigma_l^- = 2 + 2\sigma_l^z, \qquad \sigma_l^-\sigma_l^+ = 2 - 2\sigma_l^z. \tag{3.2}$$

We take a commutator of (3.1) with H, and use (3.2). All terms containing three σ are dropped, and only the constant term of $\sigma^+\sigma^-$ or $\sigma^-\sigma^+$ is retained. The latter means that some terms

like $\sigma_i^+ \sigma_{i+1}^z$ which may break up one pair in the ground state are also dropped. Their retention proves rather awkward. Hence the linearized equation we are going to get is more restrictive than one pair break-up approximation. This also means that the calculation does not have any variational character. With these remarks we may write down the equation

$$[[\sigma_i^+, H], H] = 2J^2[2\sigma_i^+ - (\sigma_{i+1}^+ + \sigma_{i-1}^+) + \tfrac{1}{2}\sigma_i^+ - \tfrac{1}{4}(\sigma_{i+2}^+ + \sigma_{i-2}^+)]. \tag{3.3}$$

The equations for σ_i^z and σ_i^- are obtained by replacing σ^+ by σ^z and σ^- throughout, respectively. Take the matrix element of both sides of (3.3) between an exact eigenstate ψ of excitation energy $\hbar\omega$ and the ground state Ψ_0^+. Let

$$\langle \psi | \sigma_l^+ | \Psi_0^+ \rangle = f(l). \tag{3.4}$$

Then ω is determined by the appropriate equation

$$\hbar^2\omega^2 f(l) = 2J^2\ [2f(l) - \{f(l+1) + f(l-1)\} + \tfrac{1}{2}f(l) - \tfrac{1}{4}\ \{f(l+2) + f(l-2)\}]\ . \tag{3.5}$$

The solution is obviously

$$f(l) = \exp(\mathrm{i}\, kl) \tag{3.6}$$

k being determined by the periodic boundary condition, and

$$\frac{\hbar^2\omega^2}{2J^2} = 2(1 - \cos k) + \tfrac{1}{2}(1 - \cos 2k). \tag{3.7}$$

The same eigenvalue is obtained from the σ^z and σ^- equations. The result is expected to be fair only for very low energy and for small k, Hence

$$\hbar\omega \simeq 2J|k|. \tag{3.8}$$

If one applies the same method to the Hamiltonian (1.1), one gets

$$\hbar\omega = 1{\cdot}414\, J|k| \tag{3.9}$$

compared with the exact result $\hbar\omega = \pi J|k|$ and the spin-wave result $\hbar\omega = 2J|k|$. In contrast to the spin wave theory, however, we get all the three states of spin 1, and they are degenerate in energy. The spin-wave theory gives two states with $S_z = \pm 1$; the $S_z = 0$ state is collective in character in terms of the spin-wave variables and does not appear (des Cloizeaux and Gaudin 1966). For large k values the dispersion relation (3.7) is not correct.

One can also look for solutions of (3.3) near the ground state Ψ_0^-. Here we put

$$\langle \psi | \sigma_l | \Psi_0^- \rangle = g(l) = (-1)^l \mathrm{e}^{ikl} \tag{3.10}$$

and the spectrum is

$$\hbar^2\omega^2 = 2J^2(2 + 2\cos k + \tfrac{1}{2} - \tfrac{1}{2}\cos 2k). \tag{3.11}$$

As $k \to \pi$,

$$\hbar\omega = 2J(\pi' - k), \qquad k \leqslant \pi. \tag{3.12}$$

The correct spectrum very probably has the familiar doubly periodic structure, but our approximation certainly cannot bring out the connection between the branches, one starting at $k = 0$ and another emerging at $k = \pi$.

4. Discussion

The explicit form of the ground state wave functions of (2.1) clarifies some features about antiferromagnetism, but because of the one-dimensional nature, fails to throw light

on the interesting question of long-range order. The knowledge of the wave function was obtained by direct calculation on short chains, but a more systematic method, such as the Bethe–Hulthén method for (1.1), should be found for describing the ground and excited states. Starting with the fully aligned state and studying the successive spin deviations, one gets linear equations, but the appropriate generalization of the Bethe *ansatz* is not known. Perhaps variational calculations exploiting the knowledge of $\Psi_0^{\pm}$ would yield better answers for the excited states. Because of the linear ω–k relationship near $\omega = 0$, the low-temperature thermodynamic properties would not be qualitatively different from that of the ordinary linear chain.

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