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The $S = 1$ quantum spin chain with equal Heisenberg and biquadratic exchange in a magnetic field

J B Parkinson
Department of Mathematics, UMIST, PO Box 88, Manchester M60 1QD, UK

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Abstract. The $S = 1$ quantum spin chain with equal Heisenberg and biquadratic exchange was shown by Sutherland to be integrable. In this paper the equations obtained by Sutherland are solved numerically to obtain the behaviour at zero temperature in a magnetic field. It is found that there is an additional phase change at a lower field than the spin flop field. This new phase change marks the boundary between a regime in which the ground state contains only atoms with $S^z = 1, 0$ and one in which $1, 0$ and -1 are present.

The form of the elementary excitations in the two regimes is discussed and the possibility of a similar phase change in the pure Heisenberg model is considered.

1. Introduction

In this paper results are presented for a quantum spin chain of N atoms each with spin 1 described by the Hamiltonian

$$\mathcal{H} = \sum_i [J_1(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}) + J_2(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2] - H \sum_i S_i^z \tag{1.1}$$

for the particular case $J_1 = J_2 = 1$. The quantity H is proportional to the applied magnetic field. This model is sometimes called the Schrödinger or permutation model (Schrödinger and Hamilton 1941), but for the linear chain is usually known as the Lai–Sutherland model (Lai 1974, Sutherland 1975). This system is antiferromagnetic for $H = 0$. (The choice $J_1 = J_2 = -1$ has the same eigenstates but is ferromagnetic for $H = 0$ and will not be considered explicitly.) Periodic boundary conditions are used so that $\boldsymbol{S}_{i+N} \equiv \boldsymbol{S}_i$, and N is taken as even. The square of the total spin (with quantum number S_T) and the total z-component, $S_T^z = \Sigma_i S_i^z$, both commute with $\mathcal{H}$. Translational symmetry is incorporated by means of the wavevector k.

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The Hamiltonian (1.1) with $J_1 = J_2 = 1$ can be rewritten as

$$\mathcal{H} = N + \sum_i h_i - H \sum_i S_i^z \tag{1.2}$$

where $h_i = (\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}) + (\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2 - 1$ which can be written in terms of the basis of a single interacting pair as

$$h_i = \begin{array}{c} \\ |++\rangle \\ |+0\rangle \\ |0+\rangle \\ |+-\rangle \\ |00\rangle \\ |-+\rangle \\ |0-\rangle \\ |-0\rangle \\ |--\rangle \end{array} \begin{array}{c} \begin{array}{cccccccc} |++\rangle & |+0\rangle & |0+\rangle & |+-\rangle & |00\rangle & |-+\rangle & |0-\rangle & |-0\rangle & |--\rangle \end{array} \\ \begin{bmatrix} 1 & & & & & & & & \\ & 0 & 1 & & & & & & \\ & 1 & 0 & & & & & & \\ & & & 0 & 0 & 1 & & & \\ & & & 0 & 1 & 0 & & & \\ & & & 1 & 0 & 0 & & & \\ & & & & & & 0 & 1 & \\ & & & & & & 1 & 0 & \\ & & & & & & & & 1 \end{bmatrix} \end{array} \tag{1.3}$$

showing clearly the 'permutation' nature of this Hamiltonian.

The fully aligned state will be denoted by $|0\rangle$, and has $S_T^z = N$ and energy $2N$ when $H = 0$. All other energies will be measured relative to this state. For the remainder of this section H will be taken as 0.

Because of the form of h_i, the numbers of atoms of each of the three possible types $+1, 0, -1$ are conserved. Denoting these numbers by N_1, N_0, and N_{-1} respectively and defining $M_0 = N_0 + N_{-1}$, then clearly $N_1 + N_0 + N_{-1} = N$, and $S_T^z = N_1 - N_{-1}$. The fractions N_i/N and M_0/N will be denoted n_i and m_0 respectively. The set of states with given S_T^z can be further block diagonalised into states with given $[N_1, N_0, N_{-1}]$. One feature to note is that the eigenvalues for a given set $[N_1, N_0, N_{-1}]$ are identical to those for the set $[N_0, N_1, N_{-1}]$, and for any other arrangement of the N_i, although clearly these will have different S_T^z in general.

The additional block diagonalisation can be exploited in numerical calculations of short chains. It enables chains with $N \leqslant 15$ to be diagonalised using a Lanczös technique. The results for $N = 15$ are included in the figures.

Using the Bethe *ansatz* in the limit $N \to \infty$, Sutherland obtained the following integral equations for the lowest state with a given set $[N_1, N_0, N_{-1}]$.

$$R_1(\alpha) = g(\alpha) + \int_{-B_1}^{B_1} K_1(\alpha - \beta) R_1(\beta)\, \mathrm{d}\beta + \int_{-B_2}^{B_2} K_2(\alpha - \beta) R_2(\beta)\, \mathrm{d}\beta \tag{1.4a}$$

$$R_2(\alpha) = \int_{-B_1}^{B_1} K_2(\alpha - \beta) R_1(\beta)\, \mathrm{d}\beta + \int_{-B_2}^{B_2} K_1(\alpha - \beta) R_2(\beta)\, \mathrm{d}\beta \tag{1.4b}$$

where

$$g(\alpha) = 4/(1 + 4\alpha^2)$$

$$K_1(x) = -1/\pi(1 + x^2)$$

$$K_2(x) = 8/\pi(1 + 4x^2) = (2/\pi)g(x)$$

which can be solved self-consistently for R_1 and R_2 for given values of B_1 and B_2. The parameters B_1 and B_2 are related to the N_i by

$$m_0 = \frac{1}{2\pi}\int_{-B_1}^{B_1} R_1(\alpha)\,\mathrm{d}\alpha \tag{1.5a}$$

$$n_{-1} = \frac{1}{2\pi}\int_{-B_2}^{B_2} R_2(\alpha)\,\mathrm{d}\alpha. \tag{1.5b}$$

The energy per atom $\mathscr{E}$ and magnetisation $\sigma \equiv S_T^z/N$ are given by

$$\mathscr{E} = 1 - \frac{1}{2\pi}\int_{-B_1}^{B_1} R_1(\alpha)g(\alpha)\,\mathrm{d}\alpha$$

$$\sigma = 1 - \frac{1}{2\pi}\int_{-B_1}^{B_1} R_1(\alpha)\,\mathrm{d}\alpha - \frac{1}{2\pi}\int_{-B_2}^{B_2} R_2(\alpha)\,\mathrm{d}\alpha.$$

The absolute ground state of the system in zero field is the state in which $n_1 = n_0 = n_{-1} = \frac{1}{3}$, $B_1 = B_2 = \infty$, and energy $\mathscr{E} = 1 - \pi/(3\sqrt{3}) - \ln 3 = -0.70321$.

2. Effect of the magnetic field

Since S_T^z is a constant of the motion the eigenstates are unchanged by the presence of the field although clearly the eigenvalues are shifted by an amount $-HS_T^z$. For $H \geqslant H_{sf}$, where $H_{sf} = 4$ is the spin–flop field, the aligned state $|0\rangle$ is the lowest state and the magnetisation $\sigma = 1$. However, for fields in the range $0 < H < H_{sf}$, the so-called spin–flop regime, the lowest state will be one with intermediate magnetisation $0 < \sigma < 1$.

To determine how σ varies with field it is necessary to solve equations (1.4*a*, *b*) numerically. This is done by dividing the range of integration into a large number (typically 50) of intervals thus converting the integral equations into difference equations which can then be solved by matrix inversion. First a value of σ is selected. B_2 is chosen arbitrarily, B_1 adjusted to give the selected σ and the energy calculated. The process is repeated for various values of B_2 until the state of lowest energy for the given σ is obtained. A curve can then be constructed of energy versus σ for $H = 0$ the gradient of which gives the corresponding value of H for this value of σ in the spin–flop regime.

The results are shown in figures 1–3. The most notable feature is the phase change at σ_c which is numerically equal to 0.5562. For values of $\sigma > \sigma_c$, the lowest state is one in which B_2 is zero. This is a state in which only atoms with zero or one deviation are present, i.e. $N_{-1} = 0$. The value of the field H_c at which the phase change occurs is found numerically to be 0.9414. As σ decreases from σ_c the fraction n_{-1} increases smoothly from 0 to $\frac{1}{3}$ at $\sigma = 0$.

If one considers states of the type found for $\sigma > \sigma_c$, in which $N_{-1} = 0$, then it is easy to show that these states have a $1 - 1$, onto mapping to states of an isotropic $S = \frac{1}{2}$ Heisenberg chain (Bader and Schilling 1984). Consequently the magnetisation curve for this region is identical to that of the spin-$\frac{1}{2}$ system obtained by Griffiths (1964), except that it is shifted by an constant equal to $\frac{1}{2}$.

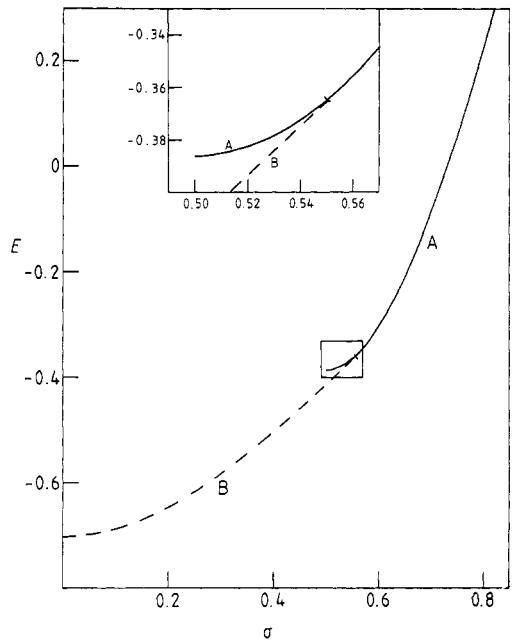

Figure 1. Curve A shows the minimum energy as a function of σ of states with $N_{-1} = 0$. The ground state is of this form for $\sigma \geqslant \sigma_c$. Curve B shows the minimum energy of states with $N_{-1} \neq 0$, giving the ground state for $\sigma < \sigma_c$. The two curves intersect tangentially at σ_c as shown in the inset. The gradient of the curves is proportional to the magnetic field for a given σ as shown in figure 2.

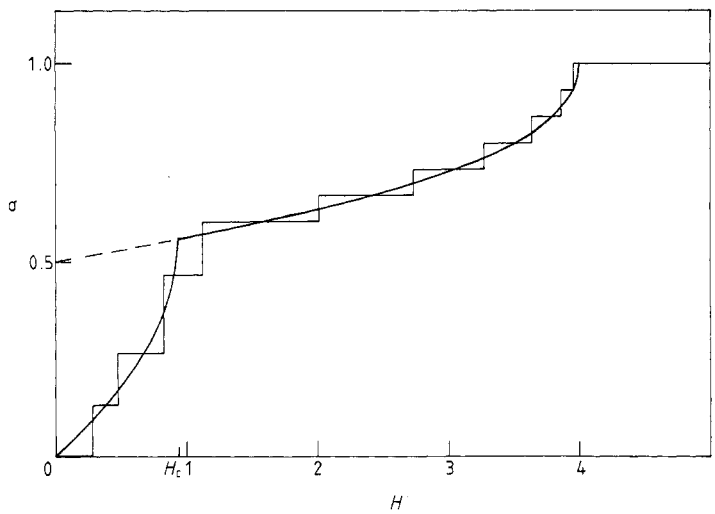

Figure 2. Magentisation curve, σ versus H. The stepped curve is the result for a chain with $N = 15$. The broken curve is the analytic continuation of the curve for $\sigma \geqslant \sigma_c$ to the region $\sigma < \sigma_c$. This curve is identical to that of the $S = \frac{1}{2}$ Heisenberg model but with a vertical shift of 0.5.

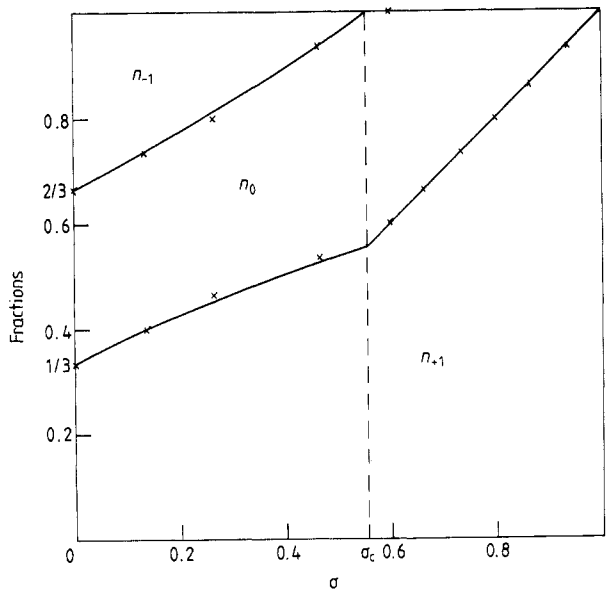

Figure 3. Variation of n_{-1}, n_0, n_1 with σ. The crosses are the values for the $N = 15$ chain.

3. Elementary excitations

The form of the elementary excitations in the spin–flop phase of an antiferromagnetic quantum spin chain is known to consist of tracking soft modes. These have a periodicity in k-space which reflects that in real space. For a spin-$\frac{1}{2}$ isotropic Heisenberg chain the modes were studied by Ishimura and Shiba (1977), who found a single soft mode. The results were later extended (Aghahosseini and Parkinson 1980) to show the full periodicity. The periodicity in real space can be visualised as consisting of atoms with a single deviation equally spaced in a background of atoms with no deviations. As the magnetic field increases towards H_{sf} the number of deviations decreases, the spacing of them in real space increases, and the periodicity in k-space decreases.

The details of these calculations are rather complicated and so they have not been carried out for the present system. Nevertheless, it is possible to predict the main features for the two distinct regimes as follows.

If $\sigma > \sigma_c$ then the behaviour will be identical to the spin-$\frac{1}{2}$ behaviour. The periodicity in k-space does not go to π as $\sigma \rightarrow \sigma_c$ since σ_c is greater than $\frac{1}{2}$.

If $\sigma < \sigma_c$ then atoms of all three types are present and the periodicity in real space is more complicated. There will be more atoms with $S_i^z = 1$ than any other type, and these can be regarded a forming the background. The standard method of obtaining the energies of the elementary excitations from the Bethe *ansatz* equations is to alter one of the quantum numbers, in the manner first described by des Cloiseaux and Pearson (1962). In the present case there are two possible ways of doing this, corresponding to introducing a discontinuity into either of the two integrals in each of equations (1.4*a*, *b*). The first integral is associated with the set of all atoms with $S_i^z = 0, -1$. There are $M_0 = N_0 + N_{-1}$ of these so if they were equally spaced the spacing would be $1/m_0$. The corresponding periodicity in k-space would be $2\pi m_0$. The second integral is associated

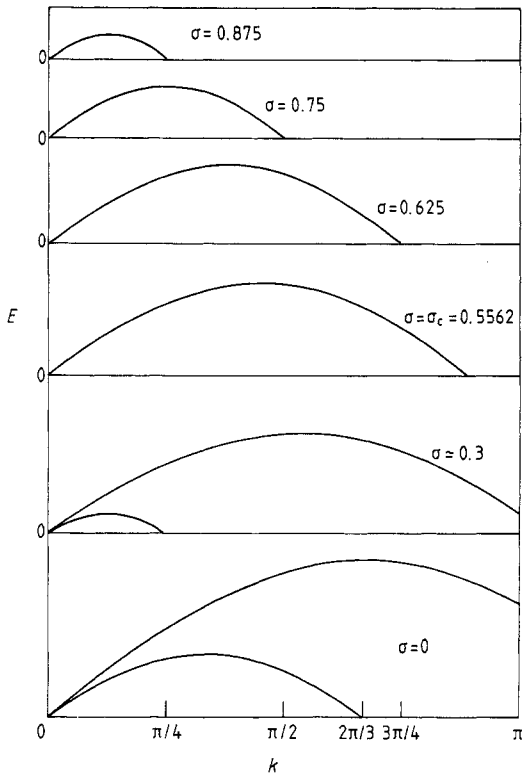

Figure 4. Spectra of elementary excitation (schematic) for various values of σ. There are two branches for $\sigma < \sigma_c$. Only the first period of each branch is shown.

only with the N_{-1} atoms with $S_i^z = -1$, so the spacing would be $1/n_{-1}$, and corresponding periodicity $2\pi n_{-1}$.

It is convenient to measure the energies of the excitation spectra relative to the lowest state with the same S_T^z. This ensures that the minima of the spectra are at zero energy. If the energies were measured relative to the lowest state with a value of S_T^z one less then there would be a gap in spectra with magnitude proportional to the magnetic field H. The amplitude of the spectra increases with the periodicity in k-space.

For $H = 0$ the two branches of the spectra are given by Sutherland as

$$\mathscr{E}_p(k) = 2\pi[\cos(p\pi/3 - k) - \cos(p\pi/3)]/3\sin(p\pi/3 - k)$$

where $p = 1, 2$. These have amplitudes $2\pi/(3\sqrt{3})$, $2\pi/\sqrt{3}$ and periodicities $2\pi/3$, $4\pi/3$ respectively.

Figure 4 shows a schematic picture of the excitations for various values of σ.

4. Relation to the pure Heisenberg spin-1 model

An important reason for studying Hamiltonians of the form (1.1) for various values of J_1 and J_2 is that they help to shed light on the behaviour of the pure Heisenberg $S = 1$ chain (i.e. with $J_2 = 0$). In particular the question of the nature of the ground state of

the pure Heisenberg model has been of great interest following the initial work of Haldane (1983a, b). An example of how study of a related model gives useful information is the work of Affleck *et al* (1987) on the valence bond model, corresponding to the choice $J_2 = J_1/3$. (See also Arovas *et al* 1988.)

The results presented in this paper are not directly related to the question of the ground state of the pure Heisenberg model. They may, however, shed some light on the behaviour of the elementary excitations in the spin–flop phase. For the pure Heisenberg model, which is not Bethe *ansatz* integrable, these excitations have been studied numerically (Parkinson and Bonner 1985). The results are similar to the Lai–Sutherland model in that there is evidence for two phases, with a division at $\sigma_c \simeq \frac{1}{2}$. There is, however, one important difference.

In both the pure Heisenberg and Lai–Sutherland cases, the phase $\sigma_c \leqslant \sigma < 1$ shows quantum behaviour, characterised by a tracking soft mode. In the Lai–Sutherland model the phase $0 < \sigma \leqslant \sigma_c$ also shows quantum behaviour, albeit of a slightly more complicated form. For the pure Heisenberg model the numerical results for the the low-σ phase indicate a *classical* behaviour. Nevertheless, the existence of two distinct phases, separated by a critical field, in the Lai–Sutherland model does give support to the existence of two phases in the pure Heisenberg model. Whether the two phases are separated by a definite critical field in the pure Heisenberg model is still not clear, of course.

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