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LETTER TO THE EDITOR

Gapless excitations in the spin-1 bilinear-biquadratic chain

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Abstract. The susceptibility and real part of the structure factor have been calculated for the spin-1 bilinear-biquadratic chain using Trotter–Suzuki decomposition and transfer matrix methods. The results indicate an extended region around the Lai–Sutherland point where the excitations are gapless. This result is in agreement with direct diagonalization for small clusters but is in conflict with a recent spin-wave analysis.

The Hamiltonian of the bilinear-biquadratic chain has the form

$$H = \sum_{i=1}^{n-1} [\cos\theta (s_i \cdot s_{i+1}) + \sin\theta (s_i \cdot s_{i+1})^2] \tag{1}$$

where $\{s_i\}$ are spin-1 operators and the coupling parameter θ is in the range 0 to 2π.

This model has attracted considerable interest since Haldane's original conjecture concerning the possible existence of an excitation gap in spin-1 antiferromagnets [1]. Hamiltonian 1 is antiferromagnetic in the region $-3\pi/4 < \theta < \pi/2$ with a singlet ground-state, outside this region it is ferromagnetic. There are a number of specific values of θ for which the exact ground-state properties of equation (1) are known. Amongst these are two values which are of concern here. These are $\theta = \tan^{-1}(1/3)$ where the ground-state is a valency-bond solid (VBS) and there is an excitation gap [2], and $\theta = \pi/4$ where the ground-state can be found by Bethe ansatz and there are gapless excitations with soft modes at momentum 0, and $\pm\frac{2}{3}\pi$. This latter point is often referred to as the Lai–Sutherland point (LS) [3].

Away from these two points and in the range $\tan^{-1}(1/3) < \theta < (\pi/2)$ there is less agreement on the nature of the ground-state and gap with differing scenarios being current. Nomura and Takada [4] built on the result of the softmode at $2\pi/3$ found by Sutherland by proposing a triply periodic ground-state valid in the whole region $\pi/4 < \theta < \pi/2$. This ground-state essentially groups each neighbouring set of 3 spins into a singlet and hence is sometimes called a trimerized state (in analogy to a dimerized state). This state was predicted to be massive in the range $\pi/4 < \theta < \pi/2$. That is the gap closes only at each end of the interval. This picture was not completely supported by the direct diagonalization of small clusters (up to 15 spins) of Fáth and Sólyom [5]. They found evidence for the triply periodic state but no gap was detected in a region extending both above and below the LS point. More recently Xian [6] using an elegant spin wave analysis predicted a gap in agreement with Nomura and Takada. This clearly leaves the question unanswered, and it might be thought that the balance of the argument favoured the interpretation that gap is

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open at least above the LS point. However, finite cluster calculations are normally reliable. Also the approach in [4] and [6] are similar to the extent that the analysis in both cases begin with a construction of the trimerized state which is used as a ground-state ansatz. It would therefore seem useful to approach the problem using other methods.

The susceptibility and real part of the structure factor have been calculated using a Trotter–Suzuki decomposition [7] and transfer matrix methods. The details of the approach can be found in many places including [8]. The calculation was done on a long chain of length 201 sites and for Trotter dimension 5. This is a very modest value for the Trotter dimension however it is not expected that the overall qualitative picture would change for higher values, particularly in the temperature domain of the quoted results. The z-component of the susceptibility is calculated from the expression

$$\chi = \frac{T^{-1}}{n}\left\langle\left(\sum_i s_i^z\right)^2\right\rangle \tag{2}$$

where $\langle\rangle$ denote thermodynamic averaging. This quantity can be a good indicator of the non-existence of a gap for the following reason. Given that the ground-state is a singlet the first possible contribution to equation 2 can only be from higher states which occur with weight $e^{-E/T}$ where E is the energy above the ground-state. Thus if there is no gap it might be expected that χ would terminate at some finite intercept on the χ axis and if there is a gap then χ should tend exponentially to zero. This approach has been successfully used by Kubo [9].

In figure 1(a) the results are shown of a linear plot of χ against T. The label next to each curve is θ/π. Firstly consider the plot for $\theta/\pi = 1/4$ this is the LS value and is indicated by an arrow. It is seen that the data shows a broad maxima with extrapolation indicating a finite intercept on the χ-axis. This is exactly what would be expected from the know solution at this point. Now consider the plots above this line. The behaviour is identical. There is a broad maxima and a finite intercept. If a gap had opened up then it would be expected that these curves would go exponentially to zero. Other plots in this region show similar behaviour. In the region below $\theta/\pi = 1/4$ this behaviour continues to be observed. The plot for the VBS is also shown and is indicated by a double arrow on figure 1(a). This plot is seen to extrapolate to zero as expected since there is a known gap at this point. Plots lying immediately above the line $\theta/\pi = (1/\pi)\tan^{-1}(1/3)$ also appear to extrapolate to zero. These results are consistent with the gap closing at some point strictly in the range $\tan^{-1} 1/3 < \theta < \pi/4$ and remaining closed up to $\theta = \pi/2$. On figure 1(b) the data in figure 1(a) (with some additions) is shown on a log-linear plot for $\tan^{-1}(1/3) < \theta < \pi/4$. All data are shown on the same scale but the zero has been shifted so the lines are superimposed. Linearity is indicative of exponential decay of χ and the existence of a gap. The results in figure 1(b) are clearly consistent with a crossover to exponential behaviour. The general shape of these findings agree with the diagonalization of Fáth and Sólyom.

To investigate the nature of the criticality the real part of the structure factor has been calculated at momentum $2\pi/3$. This is given by

$$K = \frac{T^{-1}}{n}\left\langle\sum_{i\leqslant j}\cos\left(\frac{2\pi}{3}(j-i)\right)s_i^z s_j^z\right\rangle. \tag{3}$$

The results are shown in figure 2. For $\theta/\pi = (1/\pi)\tan^{-1}(1/3)$ and nearby values the plots are clearly curved consistent with no criticality. However for the LS point and beyond the plots appear linear and this is consistent with a triply periodic critical state.

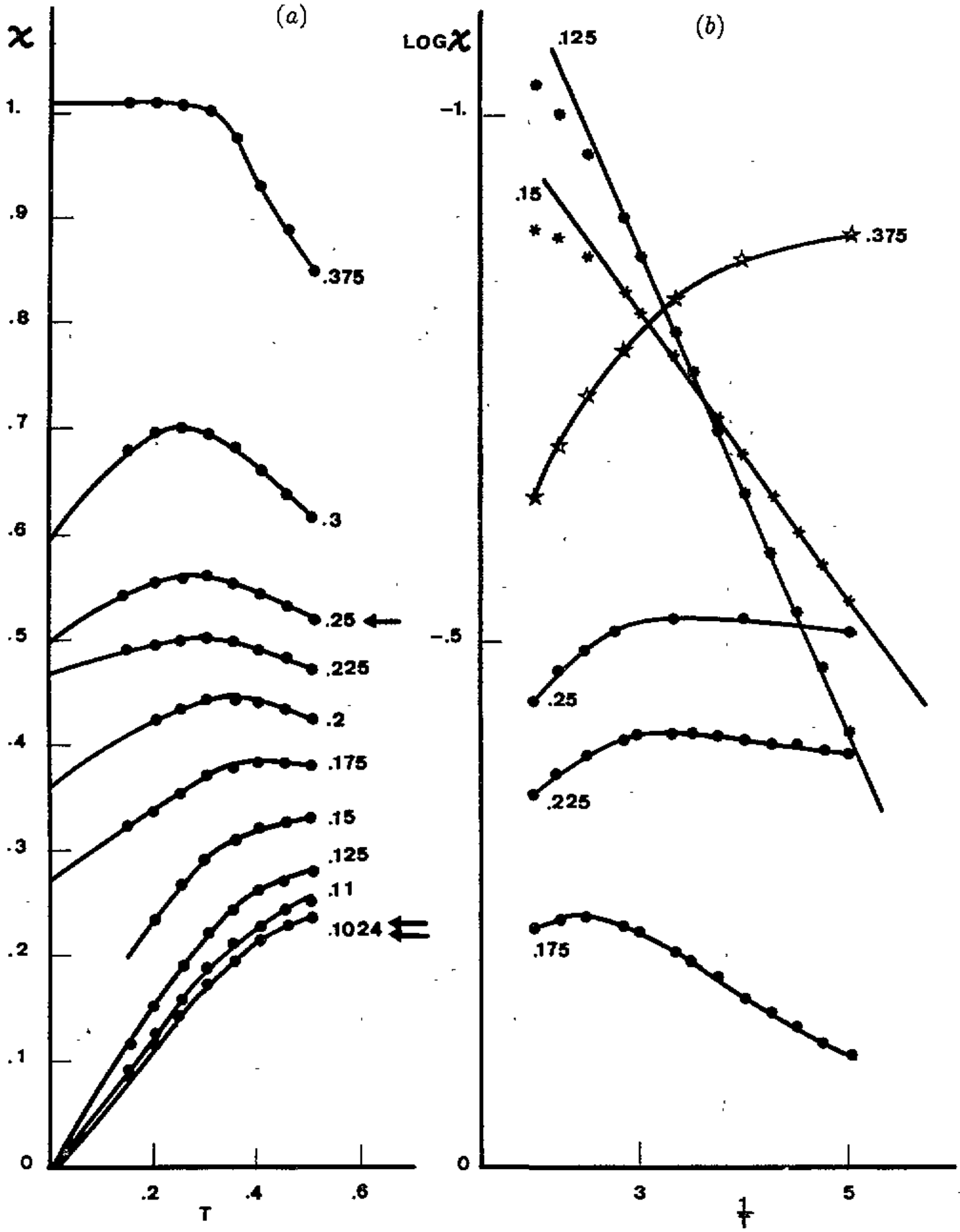

Figure 1. (*a*) Linear plot of susceptibility χ against temperature T. Numbers beside plots show value of θ/π. Single arrow (←) indicates the LS value and double arrow (⇐) the VBS value. (*b*) Log–linear plot of χ against T^{-1}. All plots use the same scale though the zeros have been shifted.

The modest value of Trotter dimension used here restricts the temperature domain of the validity of these results. However, above the LS point spin wave analysis predicts a substantial gap. Xian estimated 0.315 at $\theta = \pi/3$. Such large values, should they exist, should show a signature in the plots for χ, even in the restricted temperature domain

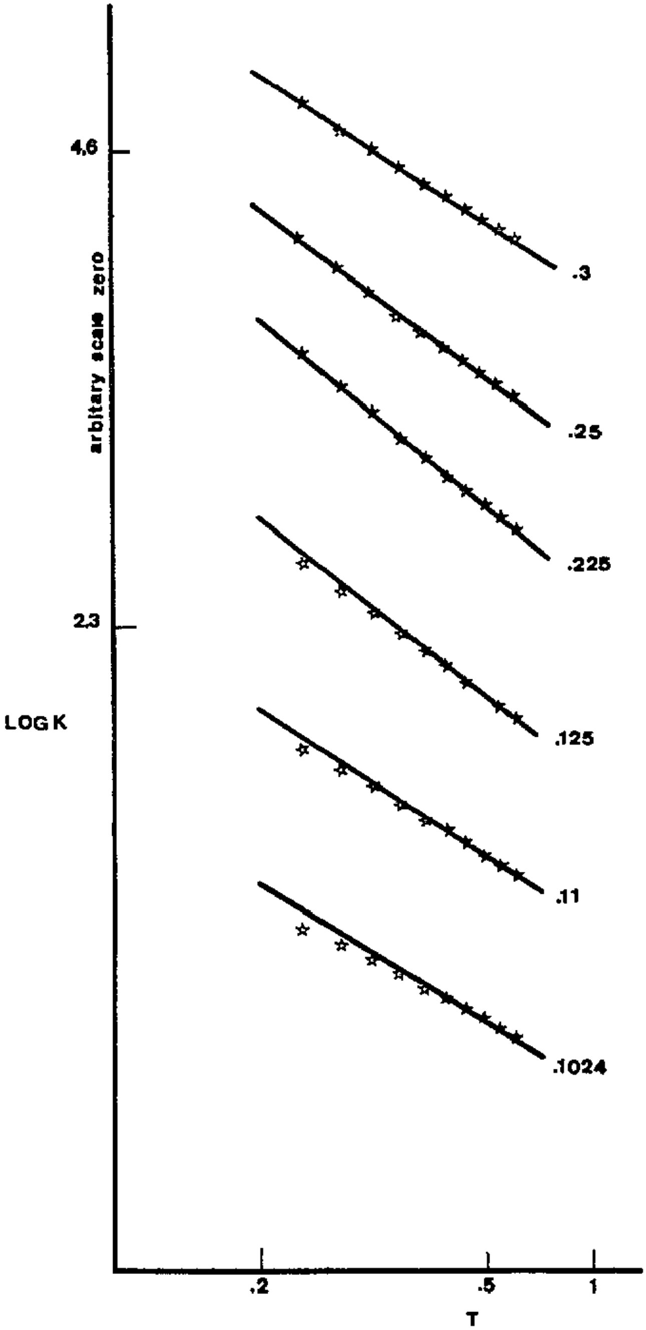

Figure 2. Log–log plot of real part of structure factor K against temperature T, at momentum $2\pi/3$. Numbers indicate the value of θ/π.

considered here. The results are thus clearly in conflict with spin wave analysis and indicate that there is no gap, though a small gap cannot be excluded. Below the LS point the situation is more subtle. Early work by Fáth and Sólyom [5] indicated that the gap was closed immediately below the LS point. However in more recent work [10] Fáth and Sólyom have concluded that the gap is exponentially small below the LS point and the transition is in the class of a Kosterlitz Thouless transition. Clearly the results reported here are consistent with both these scenarios and it would be necessary to approach much lower temperatures to be sure.

If spin wave theory fails above the LS point this may be because the perfectly trimerized state is too simple a model to describe the true ground-state. There is some evidence for this contained in the work of Bishop *et al* [11]. It could also be as Xian suggests that it is necessary to include in the analysis higher spin state with total spin exceeding 1.

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