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The statistical mechanics of the related $S = \frac{1}{2}$ anisotropic and $S = 1$ pure biquadratic quantum spin chains

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Abstract. We consider a quantum spin chain with $S = \frac{1}{2}$ and anisotropic exchange (XXZ model) with $\Delta = -\frac{3}{2}$. This integrable system has a partial mapping to an $S = 1$ chain with pure biquadratic exchange. We calculate the magnetisation curves at zero temperature which are identical for the two systems. We also use the integral equations obtained by Gaudin to study the specific heat as a function of temperature and magnetic field. The results are compared with numerical calculations for short chains of the $S = 1$ system. The maximum occurs at approximately the same position for the two systems, but the shapes of the curves differ considerably.

1. Introduction

It has recently been shown (Parkinson 1987, 1988) that a partial mapping exists between two quantum spin chains with different values of spin S. The two Hamiltonians are an $S = \frac{1}{2}$ XXZ model given by

$$\mathcal{H}_1 = J \sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z) - H \sum_i S_i^z \tag{1.1}$$

and a pure biquadratic $S = 1$ model given by

$$\mathcal{H}_2 = J_2 \sum_i (\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2 - H \sum_i S_i^z. \tag{1.2}$$

In both cases periodic boundary conditions are assumed so that $\boldsymbol{S}_{i+N} \equiv \boldsymbol{S}_i$, where N is the number of atoms in the chain. Translational symmetry is incorporated by means of the wave-vector k. The total z component $S_T^z = \Sigma_i S_i^z$ commutes with both $\mathcal{H}_1$ and $\mathcal{H}_2$, while the square of the total spin (with quantum number S_T) commutes only with $\mathcal{H}_2$. H is proportional to the magnetic field.

States of the two Hamiltonians (1.1) and (1.2) have identical energies provided $\Delta = -\frac{3}{2}$ and $J = 2J_2$, with the exception of states in which $S_T^z = 0$. The mapping between the two Hamiltonians is between 1-strings of (1.1) and 2-strings of (1.2), so states with $S_T^z = r$ of the former have the same energies as states with $S_T^z = 2r$ of the latter. The mapping is only partial, however, and for a given S_T^z there are many more states of (1.2), including those for which $S_T^z < S_T$. Nevertheless, the lowest states for each value of S_T^z and k are the same for the two Hamiltonians.

Barber and Batchelor (1989) have recently shown that states with $S_T^z = 0$ of the two Hamiltonians are the same in the thermodynamic limit, $N \to \infty$ (they actually considered

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a system without periodic boundary conditions). A similar conclusion was reached by a different method by Klümper (1989). $\mathcal{H}_2$ is antiferromagnetic for $J_2 < 0$ and ferromagnetic for $J_2 > 0$ and, although the eigenstates are the same for either sign (with different eigenvalues), J_2 will be assumed negative, and hence $J = 2J_2$ will also be negative. For convenience we shall put $J = -1$, which is equivalent to measuring H and the energies in units of $|J|$.

For $H = 0$ the ground state of (1.1) was given by Orbach (1958) and Walker (1959). It is doubly degenerate with energy $E_0 = -Nw$, where, defining $x = (7 + 3\sqrt{5})/2$

$$w = (\sqrt{5}/2)\left(\tfrac{1}{2} + 2\sum_{n=1}^{\infty}(1 + x^n)^{-1}\right) = 1.796\,864. \tag{1.3}$$

The elementary excitations were calculated by des Cloiseaux and Gaudin (1966) using the same method that des Cloiseaux and Pearson (1962) had used for the isotropic Heisenberg model (i.e. $\Delta = 1$). For $S_T^z = \pm 1$ they found a spectrum with a gap from the ground state which for $\Delta = -\frac{3}{2}$ has the value 0.173 179. The analytic form (Gaudin 1971) is

$$E_{\text{Gap}} = 2\sqrt{5}\,\text{dn}(\pi) = \sqrt{5}\,A^2 = 0.173\,179 \tag{1.4}$$

where

$$A = 1 + 2\sum_{n=1}^{\infty}(-1)^n q^{n^2} \qquad \text{with } q = (3 - \sqrt{5})/2.$$

The form of the spectrum given in their paper can be rewritten in a simpler form, by making use of the series expansions and other relations of the Jacobian elliptic functions. When this is done the result is

$$\mathcal{E}(k) = E_{\text{Gap}}\sqrt{1 + a\sin^2 k} \tag{1.5}$$

where $a = m_1/m$, using the standard notation for elliptic functions.

They also found another spectrum for $S_T^z = 0$ with identical form but no gap. The end points of this are the doubly degenerate ground state, but for all other values the results are incorrect. They are based upon an assumption about the allowed distribution of integers in the Bethe *ansatz* equations. This distribution is not observed in short-chain calculations, using the method of Hodgson and Parkinson (1984).

2. The zero-temperature magnetisation curve

The magnetisation $\sigma \equiv S_T^z/NS$ for a given H depends only on the lowest eigenvalue for each S_T^z of the Hamiltonian and not on its degeneracy. Consequently it will be identical for (1.1) and (1.2) apart from a factor of 2 for the reasons noted above. The curve was calculated for the isotropic $S = \frac{1}{2}$ Heisenberg Hamiltonian by Griffiths (1964). We calculate it for the specific case $\Delta = -\frac{3}{2}$, using the method of Yang and Yang (1966a, b, c).

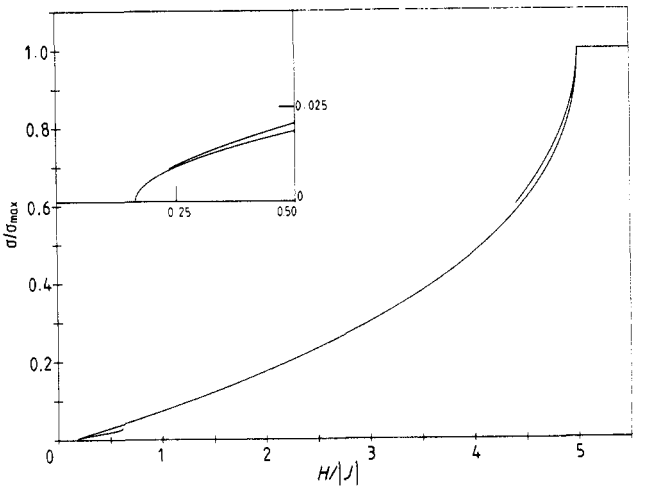

Figure 1. The magnetisation curve for both (1.1) and (1.2). The asymptotic formulae for σ close to 0 and to σ_{max} are also shown. The inset is an enlargement of the low-σ region.

The integral equation that has to be solved is

$$f_c(\xi) = g_0(\xi) - \int_{-c}^{c} K(\xi, \eta) f_c(\eta)\, \mathrm{d}\eta \tag{2.1}$$

where $g_0(\xi) = (2/\pi)(1 + \xi^2)^{-1}$,

$$K(\xi, \eta) = \frac{2}{\pi} \frac{1 - \frac{1}{2}\alpha(1 - \eta^2)}{[2 - \alpha(1 - \eta\xi)]^2 + (\xi - \eta)^2}$$

and $\alpha = 1 - 1/\Delta$. The parameter c is related to the magntisation σ by $\sigma = 1 - \rho$ with

$$\rho = \tfrac{1}{2} \int_{-c}^{c} f_c(\xi)\, \mathrm{d}\xi$$

and the energy is given by

$$\mathscr{E} = \frac{\pi}{2} \int_{-c}^{c} [(1 - \alpha) g_0(\xi) + \alpha/\pi] f_c(\xi)\, \mathrm{d}\xi. \tag{2.2}$$

The corresponding magnetic field is obtained from the equation

$$H = 3\, \mathrm{d}\mathscr{E}/\mathrm{d}\rho. \tag{2.3}$$

The procedure in practice involves choosing a value of c, determining $f_c(\xi)$ from (2.1), then evaluating the corresponding values of σ and H. The integral equation is solved numerically by dividing the range into 300 equal intervals, thus converting it to a matrix equation. The result is shown in figure 1.

There are two critical fields: $H_{SF} = 5$ is the spin-flop field at which the magnetisation reaches its maximum value $\sigma = 1$, and $H_c = E_{Gap}$ is the field at which σ becomes 0. For

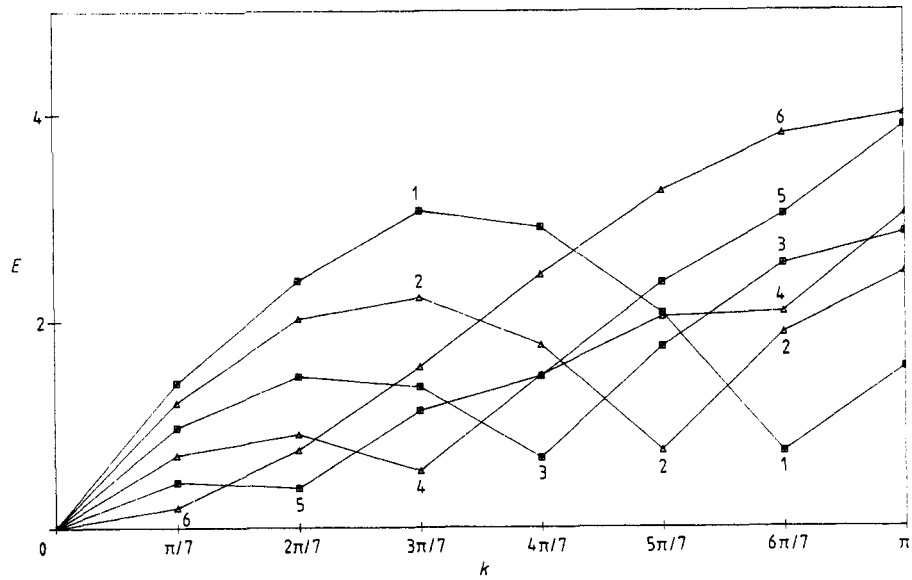

Figure 2. The tracking soft mode for a chain of 14 atoms for (1.1). Curves are labelled with the values of S^z_T. Equations (1.2) are identical apart from a factor of 2 in the values of S^z_T.

σ close to 1 a simple spin-wave approximation gives $H \simeq 5 - (3\pi^2/8)(1-\sigma)^2$. For σ close to 0 the asymptotic expression is given by Yang and Yang as

$$H = 2\sqrt{5}[e_0 + (4\pi^2 e_2/e_0^2)\sigma^2 - (64\pi^3 e_2 f_0/3e_0^3)\sigma^3 + \ldots]$$

$$H = E_{\text{Gap}} + (6.35 \times 10^3\sigma^2 - 5.43 \times 10^5\sigma^3 + \ldots)$$

where

$$e_0 = \text{dn}(\pi) \qquad e_2 = (mK^2/2\pi^2)e_0 \qquad f_0 = w/(\sqrt{5}\pi).$$

Both these limiting cases are shown on the figure.

3. The spectrum for $H \neq 0$

The elementary excitations at $T = 0$ in the presence of a field fall into three categories. For $H < H_c$ there is a gap equal to $H_c - H$, but otherwise the spectrum is the same as at $H = 0$. For $H_c \leqslant H \leqslant H_{SF}$ the spectrum is gapless and exhibits a tracking soft mode (Beck *et al* 1981). For $H > H_{SF}$ there is again a gap, equal to $H - H_{SF}$ and the form of the spectrum above this gap is the usual ferromagnetic spin-wave spectrum.

The most interesting region is the gapless one. The tracking soft mode has a zero at wave-vector $k^* = (1-\sigma)\pi$. Such a mode was first predicted by Ishimura and Shiba (1977) for the $\Delta = 1$ case. In fact the spectrum is periodic with this period (Aghahosseini and Parkinson 1980). For $|\Delta| > 1$ the spectrum is slightly different, in that minima for successive values of S^z_T always occur at $k = 0$ instead of alternating between $k = 0$ and $k = \pi$. This is connected with the fact that S_T is no longer a good quantum number.

Calculation of the details of the spectrum in this region is rather complicated and we have not carried it out. The phenomenon can be observed in short chains, although for finite N the soft mode does not come down to zero. In figure 2 we show the lowest

energies for each S_T^z for a chain of 14 atoms for (1.1), relative to the corresponding energy at $k = 0$. For (1.2) the same spectrum occurs for even values of S_T^z, with a factor of 2 in these values, but the spectrum for odd values has additional features (see Parkinson 1988).

4. Non-zero-temperature properties

The anisotropic $S = \frac{1}{2}$ Hamiltonian (1.1) can be analysed at non-zero temperature in terms of strings, using the method originally pioneered for 1D magnets by Takahashi (1971). For (1.1) the relevant equations were given by Gaudin (1971) (see also Johnson 1974). The low-temperature behaviour for all Δ and H was thoroughly analysed by Johnson and McCoy (1972) and numerical solutions for some values of Δ and H over the whole temperature range were given by Johnson (1974). We have solved the equations numerically for the specific case $\Delta = -\frac{3}{2}$ for various H.

In addition, numerical results for short chains ($N \leqslant 14$) can be obtained by direct diagonalisation of the Hamiltonian, and these were used to verify the numerical solution of the integral equations for higher T. This second method of direct diagonalisation is the only method available for studying (1.2) for $T \neq 0$, since the mapping between the two Hamiltonians is only partial.

The integral equations, which have to be solved self-consistently for the variables $\varepsilon_n(\phi)$, are

$$\varepsilon_n/T = \mathrm{Dn}*\{\ln([1 + \exp(\varepsilon_{n+1}/T)][1 + \exp(\varepsilon_{n-1}/T)])\} \qquad n > 1 \tag{4.1a}$$

$$\varepsilon_1/T = \mathrm{Dn}*\{\ln[1 + \exp(\varepsilon_2/T)]\} - T^{-1} \sinh \Phi \, \mathrm{Dn}(\phi) \tag{4.1b}$$

where $\cosh \Phi = |\Delta|$ and $\mathrm{Dn}(\phi) \equiv (K/\pi)\,\mathrm{dn}(K\phi/\pi, m)$ with $K/K' = \pi/\Phi$, using the usual notation for the elliptic function (Abramowitz and Stegun 1964). The convolution Dn* is defined as

$$\mathrm{Dn}*\{\rho(\phi)\} \equiv \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{Dn}(\phi - \phi')\rho(\phi')\,\mathrm{d}\phi'. \tag{4.2}$$

The coupled equations are completed by taking the asymptotic limit

$$\lim_{n\to\infty} \frac{\varepsilon_n}{T} = \ln(\gamma_n^2 - 1) \tag{4.3}$$

where

$$\gamma_n = \begin{cases} n + \text{constant} & H = 0 \\ \dfrac{\sinh(nH/2T + \text{constant})}{\sinh(H/2T)} & H \neq 0. \end{cases} \tag{4.4}$$

The constants are not strictly necessary in the limit $n \to \infty$ but greatly speed up convergence.

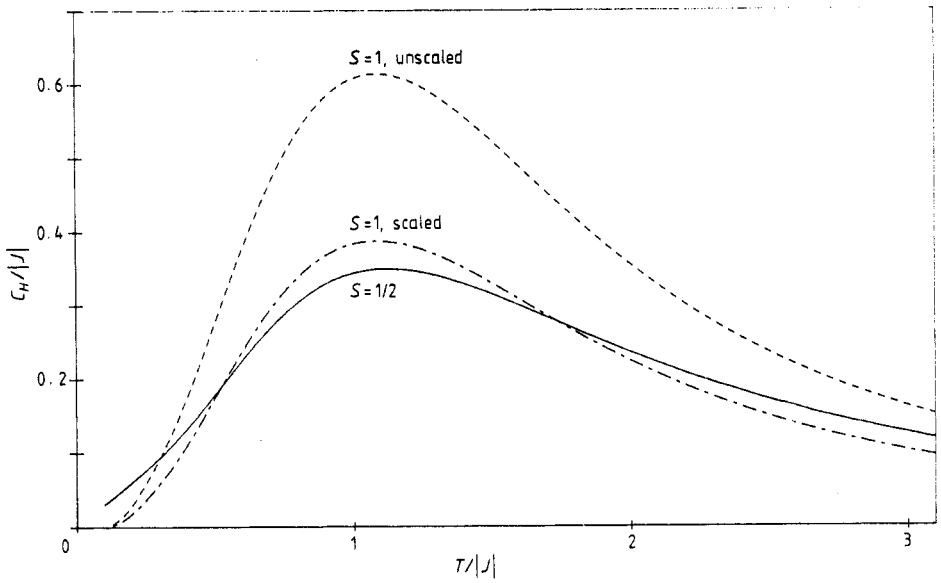

Figure 3. Specific heat curves at $H = 0$ for (1.1) and (1.2).

The free energy per atom is

$$F(T, H)/N = E_0/N - \frac{T}{2}\int_{-\pi}^{\pi} \mathrm{Dn}(\phi) \ln[1 + \exp(\varepsilon_1/T)]\, \mathrm{d}\phi + \sigma H \tag{4.5}$$

which depends explicitly only on ε_1. Differentiating with respect to H gives the magnetisation $\sigma(T, H)$. Differentiating with respect to T gives the entropy $S(T, H)$, and differentiating again with respect to T gives the specific heat $C_H(T, H)$. These differentiations were performed numerically.

The $H = 0$ results are shown in figure 3. The results for (1.1) are shown directly and also divided by a factor of $\ln(3)/\ln(2)$ in the vertical scale, which makes the area under the curves for the two Hamiltonians the same. This is because $S = 1$ has a multiplicity 3, while $S = \frac{1}{2}$ has a multiplicity 2, resulting in a factor $\ln(3)/\ln(2)$ in the entropy.

Figure 4 shows specific heat curves for $H \neq 0$. The low-temperature behaviour for $H = H_{SF}$ for the two models is very similar, which we believe reflects the fact that the low-lying excitations in both cases are 'ferromagnetic' spin waves with the same energies and degeneracies. Figure 5 shows the $T \neq 0$ magnetisation curves. The magnetisation curves for short chains are stepped at $T = 0$ and although the steps become smoothed at higher temperature the short-chain results for the susceptibility have high peaks which would not be present in the infinite chains. Nevertheless, we show the susceptibility curves in figure 6, as the final peak close to H_{SF} is clearly similar to the two models.

5. High-temperature expansions

One other method of comparing the behaviour of the two models in an analytic rather than numerical way is by means of the high-temperature asymptotic expansions. Since

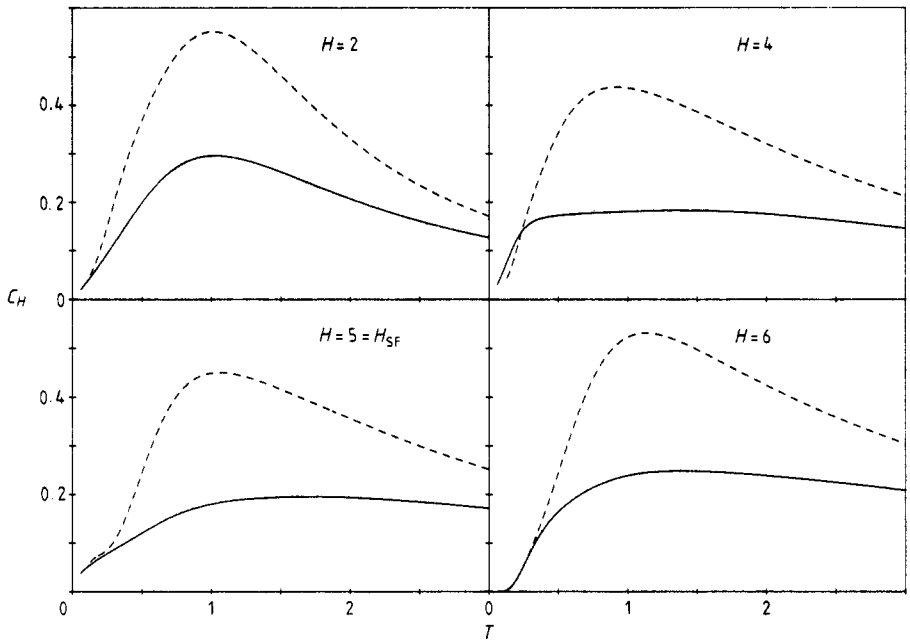

Figure 4. Specific heat curves for various H. In this and the following figures the full curve is for (1.1) and the broken curve for (1.2), while C_H, H and T are all expressed in units of $|J|$.

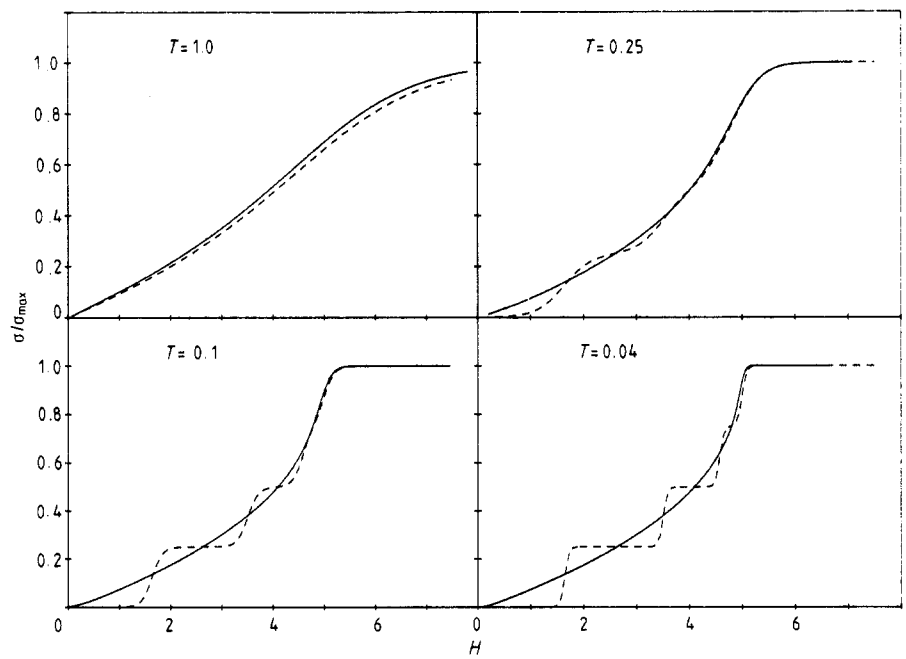

Figure 5. Magnetisation curves for various $T \neq 0$.

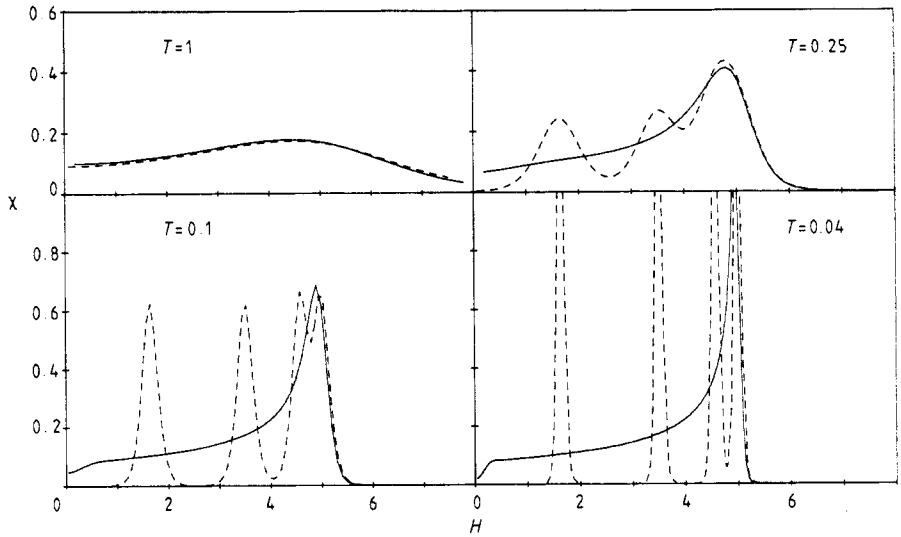

Figure 6. Susceptibility curves for various $T \neq 0$.

the $S = 1$ pure biquadratic Hamiltonian (1.2) is not fully integrable, the normal finite-temperature method used for (1.1) is clearly not available. Nevertheless, it is possible to obtain exact results for both Hamiltonians in the thermodynamic limit $N \rightarrow \infty$ in the form of an expansion in powers of T^{-1}.

For $H = 0$ the first five terms in the series for (1.1) are given by Dalton and Wood (1967) and additional terms by Wood and Dalton (1972). We have used a simple version of the same method to calculate the first two terms for (1.2) for $H = 0$.

Defining $t_2 = k_B T/|J|$ and $t_2 = k_B T/2|J_2|$, we have

$$C_H = \tfrac{17}{16} t_1^{-2} + \tfrac{9}{8} t_1^{-3} - \tfrac{213}{64} t_1^{-4} + \ldots \qquad \text{for (1.1)}$$

$$C_H = \tfrac{8}{9} t_2^{-2} + \tfrac{56}{27} t_2^{-3} + \ldots \qquad \text{for (1.2).}$$

For $H \neq 0$, only the leading term for $S = \frac{1}{2}$ Hamiltonian has been obtained:

$$C_H = (\tfrac{17}{16} + H^2/4) t_1^{-2} + \ldots .$$

These results are only valid at temperatures considerably higher than those shown in the figures, so they have not been displayed.

6. Conclusions

The $S = \frac{1}{2}$ XXZ model with $\Delta = -\frac{3}{2}$ can be studied in great detail using the full power of the Bethe *ansatz*. Probably the only important quantity that is not available via this method is the correlation function. Because of the partial mapping to the $S = 1$ pure biquadratic model, some quantities are identical for the two systems, in particular the zero-temperature magnetisation curve and the spectrum of elementary excitations.

We have found that non-zero temperature properties of the two systems are different. The differences are most marked for the specific heat, where the $S = 1$ curve is much broader, although the maximum is in approximately the same place. This

indicates that the density of states is less peaked, but covers a similar range of energies, as would be expected from the existence of the partial mapping. The magnetisation curves at non-zero temperature are not very different, and again this indicates that the low-lying states for each S_T^z have similar energies.

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