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Thermodynamics of a spin-S' impurity in a spin-S antiferromagnetic Heisenberg chain

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Abstract. The numerical solution of the Bethe *ansatz* equations of an integrable SU(2)-invariant generalization of the spin-S antiferromagnetic Heisenberg chain (Takhtajian–Babujian model) with a spin-S' impurity in zero magnetic field is presented. The entropy, specific heat and susceptibility of an impurity of spin S' are obtained numerically as a function of the spin S of the chain. Three situations have to be distinguished: (i) if $S' = S$ the impurity just corresponds to one more site in the chain; (ii) if $S' > S$ the impurity spin is only partially compensated (undercompensated) at $T = 0$, leaving an effective spin of $(S' - S)$; (iii) if $S' < S$ (overcompensated) the entropy has an essential singularity at $T = h = 0$, giving rise to critical behaviour as h and T tend to zero. These properties are in close analogy with those of the n-channel Kondo problem. The thermodynamics of the two models is compared.

1. Introduction

The isotropic spin-$\frac{1}{2}$ antiferromagnetic Heisenberg chain was first diagonalized by Bethe [1]. The standard extension of the Heisenberg chain to spin $S > \frac{1}{2}$ is unfortunately not integrable. However, an integrable SU(2)-invariant generalization of the isotropic chain of arbitrary spin S has been diagonalized [2–6] and its thermodynamics has been obtained. Even though this model is different from the standard extension of the Heisenberg model to arbitrary spin S, it is expected that its low temperature properties are similar and it has received attention in the literature.

The SU(2) generalization of the standard Heisenberg model (Babujian–Takhtajian model [6, 3]) is given by

$$H = J\left(\sum_{i=1}^{N} Q_{2S}(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}) - E_{\mathrm{vac}}\right) - h\sum_{i=1}^{N} S_i^z \tag{1.1}$$

where E_{vac} is such that the interaction energy of the state with all spins S parallel vanishes, h is the magnetic field, N is the number of lattice sites, and $Q_{2S}(X)$ is given by

$$Q_{2S}(X) = \sum_{j=1}^{2S}[\psi(j+1) - \psi(1)] \prod_{l=0,\neq j}^{2S} \frac{X - X_l}{X_j - X_l} \tag{1.2}$$

with

$$X_l = \tfrac{1}{2}[l(l+1) - 2S(2S+1)]. \tag{1.3}$$

Here ψ is the digamma function. The antiferromagnetic case is obtained by taking the coupling constant $J = 1$. The ferromagnetic case corresponds to $J = -1$. We will take $J = 1$ in the rest of the paper.

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The SU(2)-invariant spin chains remain integrable if a link to an impurity site is added to the chain, provided that the interaction between the impurity spin and its neighboring spins is of a special form. For a chain of spin $\frac{1}{2}$ and an impurity of arbitrary spin S' the interaction Hamiltonian was constructed by Andrei and Johannesson [7]. The case of a spin-1 chain with an impurity of arbitrary spin was also diagonalized [8] as well as that of a spin-S chain with a spin-$\frac{1}{2}$ impurity [9]. The case of a spin-S chain with an arbitrary impurity spin S' can be extended from the solutions of the previous cases [9].

Three situations have to be distinguished. (i) If $S = S'$ the impurity just corresponds to one more site in the chain and its properties are identical to those of the other spins [6]. In this case the ground state is a singlet due to the antiferromagnetic coupling. (ii) If $S' > S$ the spins of the chain are not able to compensate the impurity spin S' into a singlet at low temperatures [7, 8]. The presence of a small magnetic field completely orients the remaining effective spin $(S' - S)$ at zero temperature [9]. (iii) If $S' < S$ a perfect compensation of the impurity spin by the neighboring lattice sites cannot take place and the remaining spin degrees of freedom induce unusual physical properties. The $T = 0$ entropy has an essential singularity at $h = 0$: at $h = 0$ the ground-state entropy is finite and corresponds to a fractional spin dependent on both S and S' [9]. When $h \neq 0$ the entropy becomes zero [9]. The low-temperature low-magnetic-field thermodynamic quantities show power-law behaviour with critical exponents. The susceptibility and C/T, where C is the specific heat, diverge as h and T tend to zero. The exponents depend only on the spin of the chain and not on the impurity spin, since the critical behaviour is a consequence of the collective excitations of the lattice.

A similar behaviour has been found for the n-channel Kondo problem [10–13] with a spin S' impurity with $n = 2S$, where n is the number of orbital channels of the conduction electrons. In this model the conduction-electron spins interact antiferromagnetically with the impurity spin. If $n = 2S'$ the number of conduction-electron channels is exactly sufficient to compensate the impurity spin into a singlet, giving rise to Fermi-liquid behaviour. If $n < 2S'$ the impurity spin is only partially compensated, since there are not enough conduction-electron channels to yield a singlet ground state. This leaves an effective degeneracy (in zero field) at low temperatures of $(2S' + 1 - n)$. If $n > 2S'$ the number of conduction-electron channels is larger than required to compensate the impurity spin. The impurity shows critical behaviour [11] as in the corresponding case of the Heisenberg model.

In this paper the thermodynamic Bethe *ansatz* equations of the Heisenberg model [9] are numerically solved in zero magnetic field for $S \leqslant \frac{5}{2}$ and $S' \leqslant \frac{5}{2}$. In particular the entropy, specific heat and susceptibility are obtained and the results compared to those obtained for the Kondo model [12, 13].

In section 2 we review the thermodynamic Bethe *ansatz* equations and the numerical procedure used to solve them. The results are presented in section 3 and are compared to those obtained for the Kondo model. We conclude with section 4.

2. Bethe ansatz equations and numerical procedure

The thermodynamics of model equation (1.1) for a spin-S chain, can be obtained from the thermodynamic Bethe *ansatz* equations derived in [6]. They consist of an infinite set of non-linearly coupled integral equations for functions $\eta_k(\Lambda)$, which characterize the string excitations of order k with real rapidity Λ. A string excitation of order k represents a bound-magnon state of k magnons. A convenient representation of these integral equations is the recursion sequence

$$\ln \eta_k(\Lambda) = G * \ln[(1+\eta_{k-1})(1+\eta_{k+1})] - 2\pi(J/T)\delta_{k,2S}G(\Lambda) \qquad k = 1, 2, 3, \ldots$$
$$\eta_0 = 0 \tag{2.1}$$

where the star denotes a convolution and

$$G(\Lambda) = 1/[4\cosh(\tfrac{1}{2}\pi\Lambda)]. \tag{2.2}$$

These equations are completed by the asymptotic condition

$$\lim_{k\to\infty} \frac{1}{k}\ln \eta_k(\Lambda) = \frac{h}{T}. \tag{2.3}$$

The free energy per site of the model is given by

$$F_{2S}(T,h) = F_{2S}(0,0) - T\int_{-\infty}^{\infty} \mathrm{d}\Lambda\, G(\Lambda)\ln[1+\eta_{2S}(\Lambda)]. \tag{2.4}$$

The presence of an impurity in the chain does not affect the structure of the thermodynamic Bethe *ansatz* equations [9]. The driving term in equation (2.1) remains unaltered at $k = 2S$. The lowest-energy excitations are $2S$ magnon bound states that are characteristic of the excitations of the 'bulk'. The free energy of a spin-S' impurity is given by equation (2.4) if we replace $2S$ by $2S'$. Solving the set of equations (2.1) for all k, we can obtain the free energy of any impurity of arbitrary spin S' if we select the appropriate solution of η_k. By differentiation of the free energy we can obtain the thermodynamics of both the chain spins and an arbitrary impurity [9].

In the limits $|\Lambda| \to \infty$, the Λ dependence in equation (2.1) becomes irrelevant and the equations can be solved analytically. In this limit the driving term of the integral equations vanishes, so that this situation corresponds to a free spin (high-temperature or weak-coupling limit). Keeping Λ fixed and $T \to \infty$, the driving term can also be neglected. Since the integration kernel falls off exponentially, the functions η_k are constants in this limit and the integral equations reduce to a set of algebraic equations whose solution is fixed by the asymptotic condition equation (2.3)

$$\eta_k = [\sinh((k+1)h/2T)/\sinh(h/2T)]^2 - 1 \tag{2.5}$$

which is the expression for a free spin.

In the low-T limit the driving term becomes dominant and the lowest-energy excitations are bound-states of $2S$ magnons that travel through the chain. All other states are frozen out at very low T.

The influence of the driving term decreases with increasing k. In the large-k limit the solution for $\eta_k(\Lambda)$ asymptotically approaches the free-spin value equation (2.5) for all Λ.

For intermediate values of Λ and k the recursion sequence (2.1) has to be solved numerically. The procedure to solve the thermodynamic Bethe *ansatz* equations numerically is standard [14]. Since these equations depend explicitly on the temperature they are solved for a fixed value of T. Since the influence of the driving term decreases with increasing k we may truncate the recursion relation by replacing η_k for $k = k_c$ by the large-k free-spin limit (2.5). The numerical problem then reduces to the simultaneous solution of a finite number, i.e. k_c, of coupled integral equations. Also, the range of values of Λ is truncated at $\pm\Lambda_c$, where $\eta_k(\Lambda)$ have reached their asymptotic value (2.5). For a given pair of k_c and Λ_c we solve equations (2.1) iteratively and obtain the free energy through equation (2.4). The derivatives of the free energy are obtained numerically. The accuracy of the truncation procedure can be tested by studying the dependence on k_c and Λ_c of the free-energy derivatives.

Using this numerical procedure the thermodynamics (entropy, specific heat and susceptibility) of a spin S' impurity in a spin S antiferromagnetic Heisenberg chain in zero magnetic field is presented. The results for the thermodynamics are shown in section 3 as a function of S', S and T. The parameters used in the numerical procedure were selected to achieve an accuracy of better than one percent for the temperature derivatives and a few percent for the susceptibility and the specific heat when $S \neq S'$ for the higher spins.

3. Results

Using the numerical procedure described in the preceding section we obtained the entropy, specific heat and susceptibility as a function of temperature for $S' \leqslant \frac{5}{2}$ and $S \leqslant \frac{5}{2}$.

As already discussed in section 1, at low temperatures we have to distinguish three qualitatively different situations: (i) the undercompensated impurity, $S' > S$; (ii) the totally compensated impurity spin $S' = S$; and (iii) the overcompensated case, $S' < S$. In the high- and low-T limits the recursion sequence (2.1) can be solved analytically. It is useful to state the results obtained in these two limits since they can be used as tests for the accuracy of the numerical procedure.

In the high-temperature limit the functions η_k can be replaced by their asymptotic limit (2.5). The free energy of the impurity in this limit is given by

$$F_{2S'} = -T \ln \left\{ \left[\sinh(2S'+1)h/2T \right] / \sinh(h/2T) \right\} \tag{3.1}$$

which is the expression for a free spin S'. In this limit the impurity spin is effectively decoupled from the chain spins.

The low-T behaviour shows a richer behaviour as a function of S' and S. In the limit $T \to 0$ and finite field h, the three cases behave differently. If $S' = S$ the impurity is just one more site in the chain and its thermodynamics is the same as for the pure chain [6]. The zero-temperature zero-field susceptibility is finite indicative of a ground-state singlet:

$$\chi(T=0) = 2S/\pi^2 \tag{3.2}$$

For $S' > S$, on the other hand, we obtain [9] for small fields that at $T = 0$ the impurity has an effective spin $(S' - S)$ that is weakly coupled to the spins of the chain. Finally, if $S' < S$ the impurity is overcompensated [9] and the susceptibility diverges as $h^{-1+1/S}$ as $h \to 0$. Hence, the collective behaviour of the impurity interacting with the magnetic chain leads to critical properties. Note that the critical exponent only depends on the spin of the chain, S, and not on S' except for the restriction $S' < S$. If $S = 1$ (and $S' = \frac{1}{2}$), the field-dependent term is not a power law but in this case the susceptibility diverges logarithmically as $h \to 0$ (as for the quadrupolar Kondo effect [15, 16] and a two-level system interacting with conduction electrons in a metallic glass [17, 18]).

For the zero-temperature entropy we again have to distinguish between several cases. If $S' = S$, i.e. for the Babujian–Takhtajian model, the entropy of the ground state vanishes independently of the field:

$$S(h, T=0) = 0. \tag{3.3}$$

Hence, the ground state is a singlet, which is consistent with the result for the susceptibility, equation (3.2). For $S' > S$ we obtain [9]

$$S(h=0, T=0) = \ln[2(S'-S)+1] \qquad S(h \neq 0, T=0) = 0 \tag{3.4}$$

i.e., in zero field the undercompensated-impurity case leads to an effective spin $(S' - S)$, as discussed above. If the field is non-zero the Zeemann splitting lifts the spin degeneracy and a singlet is obtained. Finally, if $S' < S$ we have [9]

$$\begin{aligned} &S(h = 0, T = 0) = \ln\{[\sin \pi(2S' + 1)/(2S + 2)]/[\sin \pi/(2S + 2)]\} \\ &S(h \neq 0, T = 0) = 0 \end{aligned} \qquad (3.5)$$

so that the efective zero-field degeneracy is not an integer but fractional.

We review now the low-T specific heat and susceptibility of the impurity. For $S' = S$ the ground state is always a singlet. The specific heat is proportional to T at low temperatures:

$$C_S = \gamma_S T \qquad \gamma_S = 2S/(S + 1) \qquad (3.6)$$

as confirmed via conformal field theory [19]. The limits $T \to 0$ and $h \to 0$ cannot be interchanged. The point $h = T = 0$ is singular and the value of γ_S depends on the order of the limits [20]. If $S' > S$ the remaining spin degeneracy of $(S' - S)$ gives rise to a Schottky anomaly for $h \simeq T$ and the zero-field susceptibility diverges with a Curie law corresponding to an effective spin $(S' - S)$. For the overcompensated case $S' < S$, C/T and χ diverge with a power law (unless $S = 1$, and $S' = \frac{1}{2}$) in zero field as $T \to 0$ [9]:

$$C/T \simeq T^{-1+4/(2S+2)} \qquad \chi \simeq T^{-1+4/(2S+2)}. \qquad (3.7)$$

If $S = 1$ and hence $S' = \frac{1}{2}$, on the other hand, the critical exponent vanishes and the divergence is logarithmic [9]:

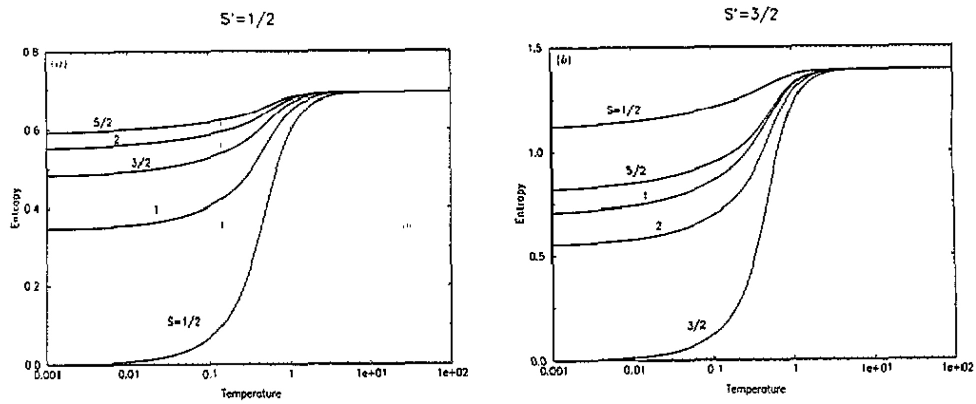
$$C/T \simeq \ln(\pi/T) \qquad \chi \simeq \ln(\pi/T). \qquad (3.8)$$

Since the field and the temperature have different scaling dimensions, $1/S$ and $4/(2S + 2)$, respectively, the limits $T \to 0$ and $h \to 0$ cannot be interchanged.

These results are in close analogy with those displayed by the n-channel Kondo model with an impurity of spin S' and $n = 2S'$ (for a review, see [21]). In this limit the integral equations (2.1) can be recast in a form that is equivalent to the thermodynamic Bethe *ansatz* equations of the n-channel Kondo model [11, 12]. In the high-temperature limit the impurity spin of the n-channel model becomes effectively decoupled from the conduction electrons, and this situation is equivalent to that observed in the Heisenberg model. Since the two limits of low and high T are equivalent in the two models it is interesting to compare their thermodynamics in the intermediate regime.

We consider now the thermodynamics in zero magnetic field using the numerical procedure discussed above. We consider first the temperature dependence of the entropy. In figure 1 we show the numerical results for $h = 0$ for three spins $S' = \frac{1}{2}$ (*a*), $S' = \frac{3}{2}$ (*b*) and $S' = \frac{5}{2}$ (*c*), as a function of T. The value at high temperatures is independent of S and is given by $\ln(2S' + 1)$, the value of a free spin S' decoupled from the chain. The crossover to the low-T regime occurs around $T = J = 1$. At low T the entropy depends on the value of S very strongly. For $S = S'$ the $T = 0$ entropy is zero due to the singlet state. If $S \neq S'$ the $T = 0$ entropy is finite due to the degeneracy of the ground state. For $S' > S$ the entropy is given by equation (3.4), corresponding to an uncompensated impurity spin $(S' - S)$. In the case $S' < S$ the $T = 0$ entropy is given by equation (3.5). This behaviour is similar to that one observed in the n-channel Kondo model [12, 13]. We note however that the high-temperature limit is reached at a temperature of the order of $T \simeq 5$–10, while in the Kondo problem this limit is only reached asymptotically. Also, the crossover regime is narrower than in the Kondo case.

In figure 2 the results for the entropy for the impurity spins $S' \leqslant \frac{5}{2}$ are shown for a given value of the spin of chain: $S = \frac{1}{2}$ (*a*), $S = \frac{3}{2}$ (*b*) and $S = \frac{5}{2}$ (*c*). The two limits



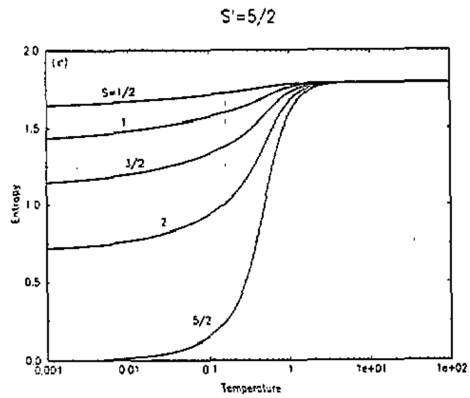


Figure 1. Entropy as a function of temperature for the chain spins $S \leqslant \frac{5}{2}$ of an impurity of spin (*a*) $\frac{1}{2}$, (*b*) $\frac{3}{2}$ and (*c*) $\frac{5}{2}$. Only when $S = S'$ is the ground-state a singlet. When $S < S'$ the entropy at zero T is that of an essentially free spin $S' - S$. When $S > S'$ the entropy corresponds to a fractional spin. In the high-T limit the entropy corresponds to a free impurity of spin S'. Note that at a temperature of the order of 10 the high-T value has been reached for all chain-spin values.

equations ((3.4) and (3.5)) are clearly shown. In the case $S = \frac{1}{2}$, the values of S' satisfy $S' > S$ (undercompensated) and the impurity entropy at $T = 0$ is given by equation (3.4). When $S = \frac{3}{2}$, the cases $S' = 2, \frac{5}{2}$ satisfy the same condition but the cases $S' = \frac{1}{2}, 1$ satisfy $S' < S$ (overcompensated). In this case the zero-T entropy corresponds to a fractional spin, equation (3.5). Note the crossing of the $S' = S = \frac{3}{2}$ curve to zero entropy due to the singlet ground-state. When $S = \frac{5}{2}$ all $S' < \frac{5}{2}$ correspond to the overcompensated case.

In figure 3 we show the specific heat as a function of T for the impurity spins $S' = \frac{1}{2}$ and $S' = \frac{3}{2}$ ((*a*) and (*b*) respectively). The specific heat is just the slope of the entropy curves multiplied by T. The peak corresponds to the Heisenberg antiferromagnetic interaction with the chain magnons. The integral of the specific heat weighed by $1/T$ gives the reduction of the entropy from the high-T value to the low-T one. The largest entropy reduction is for $S = S'$, and accordingly the peak is higher for this value of S. The peaks are centred around $T \simeq 0.4$–0.5. When $S > S'$ the height of the peak decreases with S. When $S < S'$ the height of the peak increases with S. The two cases can be found when $S' = \frac{3}{2}$ (*b*). The behaviour is similar in the Kondo model [13].

In figure 4 the ratio C/T is shown to highlight the low-T behaviour. If $S \neq S'$, C/T diverges as equation (3.7) or (3.8). In this case the model scales into a strong-coupling fixed point with a finite value of the interaction constant. A fixed point with finite coupling leads to critical behaviour and to power-law dependences in thermodynamic properties as $T \to 0$. The logarithmic divergence when $S = 1$ and $S' = \frac{1}{2}$ is clearly seen in figure 4(*a*). When $S = S'$, C/T is a constant given by equation (3.6), indicative of a singlet ground state. A similar situation is found in the n-channel Kondo problem [12, 13]. However, in

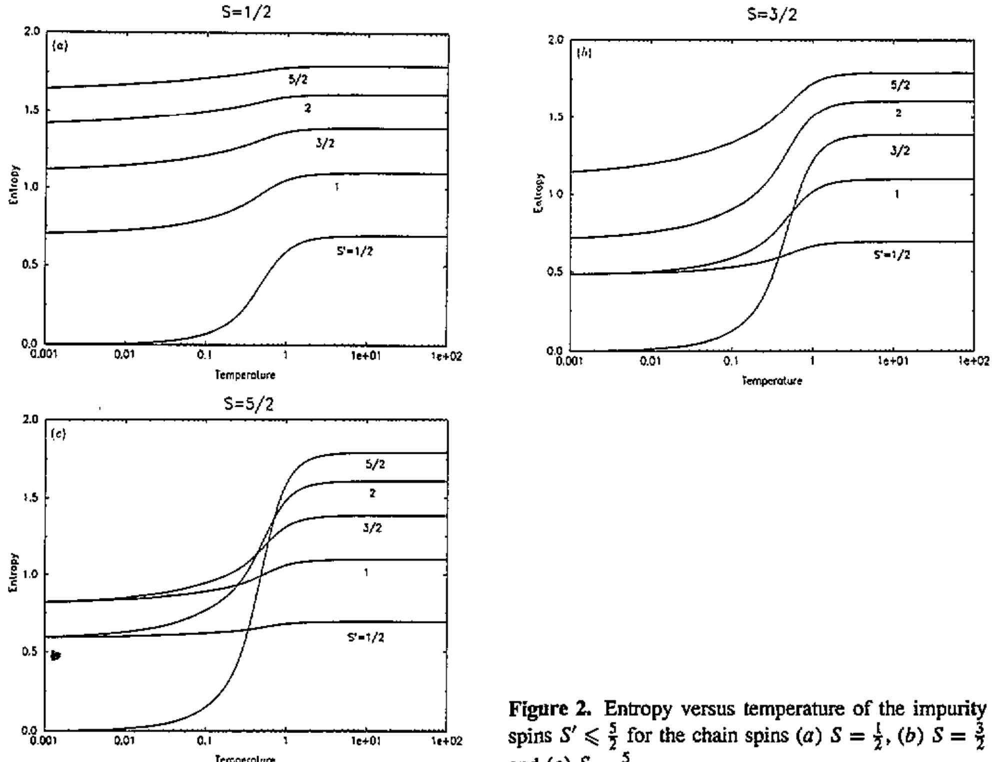


Figure 2. Entropy versus temperature of the impurity spins $S' \leqslant \frac{5}{2}$ for the chain spins (*a*) $S = \frac{1}{2}$, (*b*) $S = \frac{3}{2}$ and (*c*) $S = \frac{5}{2}$.

the intermediate-temperature regime around $T \simeq 1$, C/T for $S = S'$ shows a maximum as a function of temperature [22]. This result is in contrast to that observed in the Kondo model where C/T is monotonic. The same feature is noted for the other values of S around the same temperature. This result can be understood due to the sharper crossover from the high-temperature limit to the low-temperature limit observed in the entropy (figure 1) in comparison to the Kondo screening [22]. This implies larger values of the specific-heat peak amplitude to remove the entropy in a smaller temperature interval.

The susceptibility for the impurity-spin values $S' = \frac{1}{2}$ and $\frac{3}{2}$ is shown in figure 5(*a*) and (*b*), respectively, for values of the chain spin $S \leqslant \frac{5}{2}$. The form of these curves is similar to that found for C/T. Curie-like behaviour for a spin S' is approached at high temperatures. Note that the curves for the various values of S merge at a temperature of the order of $T \simeq$ 1–10 K. The curves show the finite value of χ for the singlet ground state for $S = S'$. Note that this curve shows a maximum as a function of temperature, as found for C/T [22]. This is again in contrast to the results obtained for the Kondo model [12, 13]. If $S > S'$, χ diverges as $T \to 0$ according to equation (3.7) or (3.8) in the case $S' = \frac{1}{2}$, $S = 1$. If $S < S'$, χ diverges with a Curie law corresponding to an effective spin $(S' - S)$. When $S \neq S'$ the curves also show a small peak around $T \simeq 1$, as when $S = S'$. This peak is especially noted when $S > S'$ (overcompensated). If $S < S'$ the susceptibility crosses smoothly over from a Curie law with a Curie constant corresponding to a spin S' at high T to another corresponding to a spin $(S' - S)$ at low T.

In figure 6 we show the susceptibility for $S' \leqslant \frac{5}{2}$ with $S = \frac{1}{2}, \frac{3}{2}$ ((*a*) and (*b*), respectively). The case $S = S'$ is noted for the finite value of χ as $T \to 0$. The cases $S' > S$ and $S' < S$ are clearly displayed. In the first case $\chi \simeq 1/T$ and in the second case χ shows critical behaviour (equations (3.7) and (3.8)). Note again the presence of the

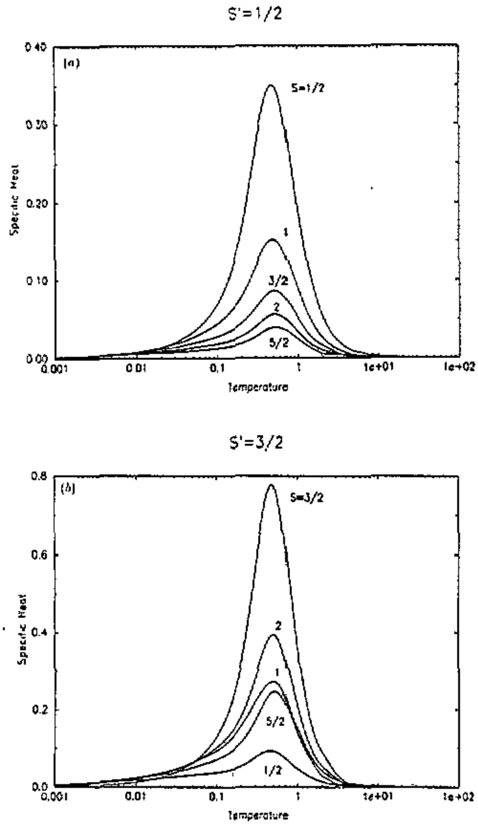


Figure 3. Specific heat for the chain-spin values $S \leqslant \frac{5}{2}$ of an impurity of spin (*a*) $S' = \frac{1}{2}$ and (*b*) $S' = \frac{3}{2}$. The highest peak is obtained when $S = S'$ since there is more entropy to be removed from the high-temperature limit to the zero-temperature value. When $S' = \frac{1}{2}$ all values of the chain spin S correspond to $S \geqslant S'$. When $S' = \frac{3}{2}$ the cases $S = \frac{1}{2}, 1$ correspond to $S' > S$ and the cases $S = 2, \frac{5}{2}$ to $S' < S$.

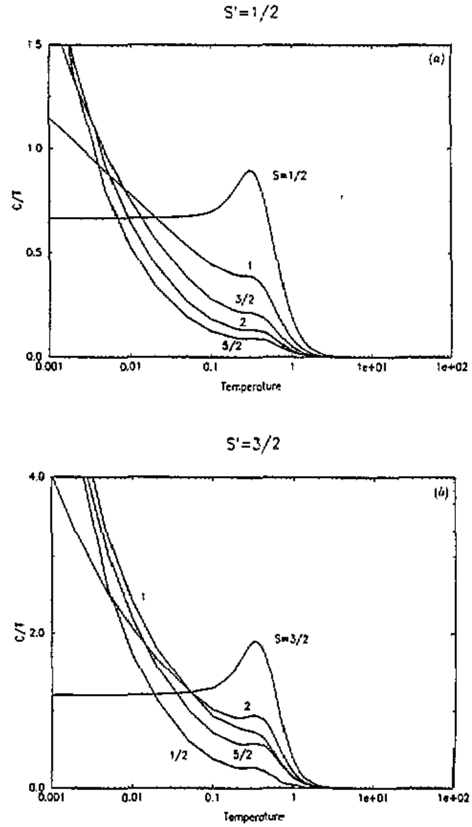


Figure 4. Specific heat over temperature versus temperature for the chain-spin values $S \leqslant \frac{5}{2}$ of an impurity of spin (*a*) $S' = \frac{1}{2}$ and (*b*) $S' = \frac{3}{2}$. When $S = S'$, C/T is finite at zero temperature and displays a maximum as a function of temperature. When $S < S'$, C/T diverges corresponding to an essentially free spin of value $S' - S$. When $S > S'$ the curve shows critical behaviour (see text). In the case of $S = 1$ and $S' = \frac{1}{2}$ the divergence is logarithmic as clearly shown in (*a*).

maximum in χ around $T \simeq 1$, especially noted for $S' < S$.

At low T and for small h the Bethe *ansatz* equations of the Heisenberg model are identical to those of the Kondo model [9]. In the presence of a field it is expected that the divergences are quenched and the low-T γ values become large but finite and constant at very low T. The same is expected for the susceptibility curves for $S \neq S'$. When $S = S'$ a small field has almost no influence. The presence of a field quenches the degeneracy of the ground state and the zero-T entropy becomes zero for all values of S and S' [9]. Similarly to the case observed in the Kondo model it is expected that the specific heat shows a double-peak structure when $S > S'$.

4. Conclusions

Exact results for the entropy, specific heat and susceptibility of the SU(2)-invariant

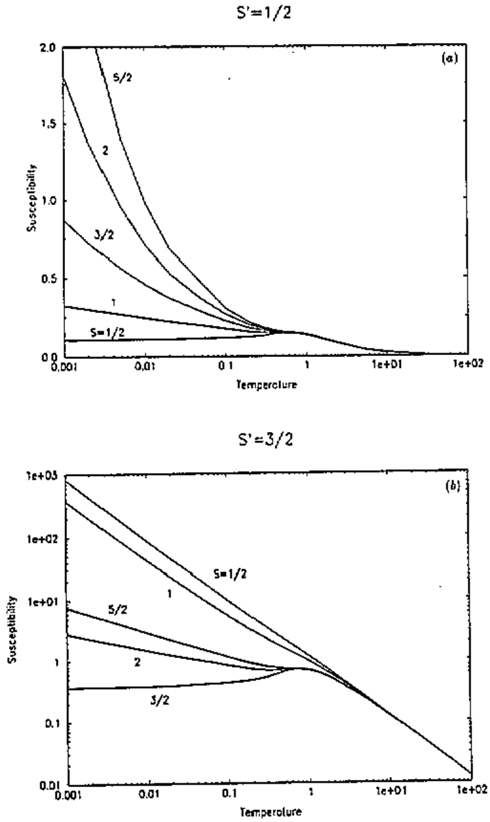


Figure 5. Susceptibility versus temperature for the chain-spin values $S \leqslant \frac{5}{2}$ of an impurity of spin (a) $S' = \frac{1}{2}$ and (b) $S' = \frac{3}{2}$. When $S = S'$ the susceptibility is finite, indicative of a singlet ground state. When $S' > S$ the behaviour is that corresponding to a free spin $S' - S$ with a Curie-like behaviour as in the high-T limit but with a modified Curie constant. When $S > S'$ the susceptibility shows critical behaviour (see text) as for the C/T curves. In the case $S = 1$, $S' = \frac{1}{2}$ the dependence in the temperature is logarithmic as can be seen in (a). Note that (b) is shown in a log–log scale.

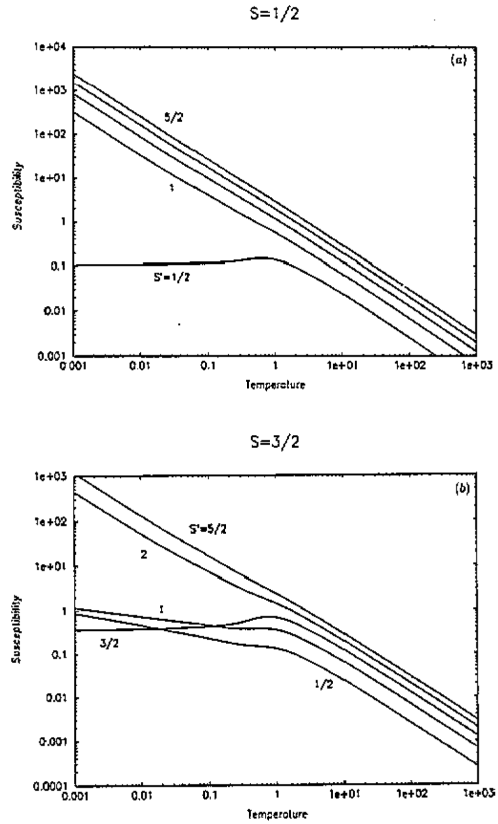


Figure 6. Susceptibility versus temperature in a log–log scale of the impurity-spin values $S' \leqslant \frac{5}{2}$ for the chain spin values (a) $S = \frac{1}{2}$ and (b) $S = \frac{3}{2}$.

antiferromagnetic Heisenberg chain of spin S with a spin S' impurity in a zero magnetic field have been obtained by solving the thermodynamic Bethe *ansatz* equations numerically [6, 9]. Three situations have to be distinguished: (i) the undercompensated impurity; (ii) the totally compensated spin; and (iii) the overcompensated impurity. The physical properties are qualitatively different for the three cases at low temperatures. When $S = S'$ the ground state is a singlet and C/T and the susceptibility are finite. When $S < S'$ the impurity behaves like a free spin with an effective spin $(S' - S)$. The case $S > S'$ is more interesting since it shows critical behaviour at low T.

The high- and the low-temperature limits of the thermodynamics of the impurity in the Heisenberg model and the Kondo model are identical. In the intermediate regime it has been found that there are notable differences between the two models when $S = S'$ [22]. In this work it was shown that the difference is also observed when $S \neq S'$. In contrast to the monotonic temperature behaviour of the susceptibility and C/T in the Kondo model, it was found that both these quantities show a local maximum as a function of temperature. When $S = S'$ this is the absolute maximum but in the cases $S \neq S'$ the low-T divergences dominate. The bump around $T \simeq 1$ is especially noted in the cases $S > S'$.

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