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Impurity-induced critical behaviour in antiferromagnetic Heisenberg chains

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Abstract. We consider an integrable SU(2)-invariant model consisting of the Heisenberg chain of arbitrary spin S (Takhtajan–Babujian model) interacting with an impurity of spin S'. The impurity is assumed to be located on the mth link of the chain and interacts only with both neighbouring sites. The starting point is a set of commuting transfer matrices, whose local weights satisfy triangular Yang–Baxter relations. The diagonalization of the transfer matrices leads to the Bethe *ansatz* equations for the model. The thermodynamics of the system is studied. 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 at $T = 0$, leaving an effective spin of $(S' - S)$. (iii) $S' < S$ 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 to those of the n-channel Kondo problem.

1. Introduction

Since Bethe's diagonalization [1] of the isotropic spin-$\frac{1}{2}$ Heisenberg chain (now known as Bethe's *ansatz*), many important properties for this model have been derived in numerous contributions [2–10]. Several integrable generalizations of the isotropic $S = \frac{1}{2}$ Heisenberg chain were found, for instance, (a) the anisotropic chain [11–13], (b) the SU(2)-invariant chain of arbitrary spin S [14–19], (c) systems of arbitrary number of components and SU(N)-symmetry [20–23], and (d) the Heisenberg chains of spin $\frac{1}{2}$ and 1 with an impurity [24, 25] of arbitrary spin S'. Some of these systems are reviewed in [26].

In this paper we extend previous results [24, 25] for impurities in a Heisenberg chain to the situation of an SU(2)-invariant chain of arbitrary spin S [15, 18] with an impurity of spin S'. We consider a chain consisting of N sites of spin S with periodic boundary conditions, i.e. a ring of length N so that $S_{N+1} \equiv S_1$. The impurity is assumed to be located on the mth link, i.e. between the mth and $(m + 1)$th sites, and interacts only with both neighbouring sites. The interaction must be of a special type [24, 25] to preserve the integrability of the model. The starting point is a set of commuting transfer matrices, whose local vertex weights ${}_{S,S'}R(\lambda)$ satisfy the triangular Yang–Baxter relations [27, 28]. This triangular relation guarantees the integrability of the system by construction. In section 2 we explicitly define the transfer matrices, show their commutative properties and diagonalize them for the special case of an impurity spin $S' = \frac{1}{2}$, but arbitrary spin S in the chain. Here we follow a similar procedure as in [14, 15, 18, 25].

The diagonalization of the transfer matrices leads to the so-called Bethe *ansatz* equations for the system. The Bethe *ansatz* equations for a general impurity spin S' are given at the end of section 2.

The thermodynamics of the system is studied in section 3. Here the excited states are classified in analogy to [6, 18] and the thermodynamic Bethe *ansatz* equations are derived. The thermodynamic properties of the impurity, in particular the small-field and low-temperature behaviour of the susceptibility and the specific heat, are presented in section 4 as a function of the impurity spin S' and the spin of the lattice S. Conclusions follow as section 5.

Our main results are the following. For the Heisenberg chain with ferromagnetic coupling the impurity, independently of its spin, is locked into the critical behaviour of the lattice, i.e. at low temperatures the specific heat is proportional to $T^{1/2}$ (ferromagnetic magnons) and the susceptibility diverges as T^{-2} with logarithmic corrections [8, 9, 19]. Three situations have to be distinguished for a chain with antiferromagnetic coupling: (i) If $S' = S$ the impurity just corresponds to one more site in the chain and consequently its properties are identical to those of the 'bulk'. (ii) If $S' > S$ the spins neighbouring the impurity are not able to compensate the impurity spin S' into a singlet at low temperatures [24, 25]. Even a small magnetic field completely orients the remaining effective spin $(S' - S)$ at zero temperature (the $T = 0$ susceptibility diverges as $H \rightarrow 0$) and a Schottky anomaly develops at finite temperatures. (iii) The most interesting case is $S' < S$. Again a perfect compensation of the impurity spin by the neighbouring 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 $H = 0$, namely it jumps from $\ln\{\sin[\pi(2S' + 1)/(2S + 2)]/\sin[\pi/(2S + 2)]\}$ at $H = 0$ to zero for $H \neq 0$, giving rise to critical behaviour in the impurity susceptibility and specific heat,

$$M(T = 0, H) \propto H^{1/S} \qquad T\chi(T, H = 0) \propto T^{4/(2S+2)} \qquad C(T, H = 0) \propto T^{4/(2S+2)} \tag{1.1}$$

so that $M(T = 0, H)/H$, $\chi(T, H = 0)$ and $C(T, H = 0)/T$ all diverge with a power law as H and T tend to zero. As expected the exponents depend only on the spin of the lattice (and not on the impurity spin, except for the condition $S' < S$), since the critical behaviour is the consequence of the collective excitations of the lattice. For the particular case $S = 1$ (and hence $S' = \frac{1}{2}$) the exponents in (1.1) are equal to 1, giving rise to logarithmic divergences [25] in χ and C/T as H and T tend to zero.

The above properties follow in almost complete analogy to those of the generalized n-channel Kondo problem [29–32].

2. Transfer matrix and the Bethe *ansatz* equations

We first have to define the vertex weight operators $R(\lambda)$, represented by matrices acting on the tensor product of two spin spaces $V_1 \otimes V_2$, $R^{j_1, j_2}_{i_1, i_2}(\lambda)$. Here j_1 and j_2 are the incoming states, while i_1 and i_2 denote the outgoing states and λ is a parameter. Integrability requires that the vertices satisfy the triangular Yang–Baxter relation

$$R^{12}(\lambda)R^{13}(\lambda + \mu)R^{23}(\mu) = R^{23}(\mu)R^{13}(\lambda + \mu)R^{12}(\lambda) \tag{2.1}$$

i.e. acting on the three-spin space $V_1 \otimes V_2 \otimes V_3$ the two processes defined by equation (2.1) yield identical results. These processes are schematically shown in figure 1.

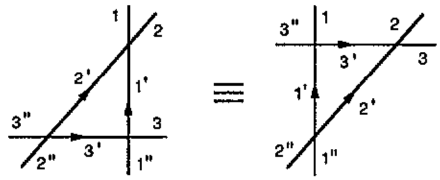

Figure 1. Schematic representation of the triangular relation, equation (2.1). On the right-hand side first particles 1 and 2 scatter, then 1 and 3 and finally 2 and 3. On the left-hand side first 2 and 3 scatter, then 1 and 3 and finally 1 and 2. The final result is the same.

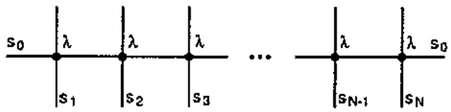

Figure 2. Schematic diagram of the monodromy matrix.

If the spins involved are all $\frac{1}{2}$, i.e. all the indices run over two states only, the non-trivial solution of equation (2.1) with SU(2) symmetry yields the well known result

$$_{\sigma}R^{12}(\lambda) = \tfrac{1}{2}(1-2\lambda)I_1 \otimes I_2 + \tfrac{1}{2}\boldsymbol{\sigma}_1 \otimes \boldsymbol{\sigma}_2 \tag{2.2}$$

where I is the identity matrix and $\boldsymbol{\sigma}$ is the vector of Pauli matrices. A transfer matrix constructed with the vertex weights (2.2) gives rise to the standard $S = \frac{1}{2}$ Heisenberg chain.

If the subspaces V_1 and V_3 correspond to a spin $\frac{1}{2}$ and the space V_2 to an arbitrary spin S, then the solution of equation (2.1) leads to (using (2.2) for $R^{13}(\lambda+\mu)$)

$$_{\sigma S}R^{12}(\lambda) = \tfrac{1}{2}(1-2\lambda)I_1 \otimes I_2 + \boldsymbol{\sigma}_1 \otimes \boldsymbol{S}_2. \tag{2.3}$$

Equation (2.3) generalizes the vertex weight (2.2) to the case where the index '1' runs over two states, while the index '2' runs over $(2S+1)$ states.

The SU(2)-invariant vertex weight for arbitrary spin S, i.e. with both indices taking $(2S+1)$ values, is obtained from equation (2.1) if the subspaces V_1 and V_3 correspond to a spin S and V_2 to a spin $\frac{1}{2}$. The vertex weight has the following form

$$_{S}R^{1/2}(\lambda) = -\sum_{j=0}^{2S}\prod_{k=1}^{j}\frac{\lambda-k}{\lambda+k}P^j \tag{2.4}$$

where P^j is a projector acting onto the space of the tensor product of the two spins involved, so that it selects the states with total spin j. In other words, if $|l\rangle$ is a state with total spin l, then $P^j|l\rangle = \delta_{j,l}|l\rangle$, and

$$P^j(x) = \prod_{\substack{l=0\\ l\neq j}}^{2S}\frac{x-x_j}{x_l-x_j} \tag{2.5}$$

$x_l = \frac{1}{2}l(l+1) - S(S+1)$. Here $x = \boldsymbol{S}_1 \cdot \boldsymbol{S}_2$, so that $P^j(\boldsymbol{S}_1 . \boldsymbol{S}_2)$ is a polynomial of order $2S$ in $(\boldsymbol{S}_1 \cdot \boldsymbol{S}_2)$. $_SR(\lambda)$ also satisfies the Yang–Baxter relation, equation (2.1), if all the spin spaces involved are of dimension $(2S+1)$.

The vertex weights for the situation where V_1 has dimension $(2S'+1)$ and V_2 has dimension $(2S+1)$ can be constructed with a similar procedure. They generalize equation (2.3) to arbitrary spins. The result for $S'=1$ and arbitrary S can be found in [25]. For the sake of clarity we consider in this section the case of a chain (with SU(2) invariance) of spins S and an impurity of spin $S'=\frac{1}{2}$.

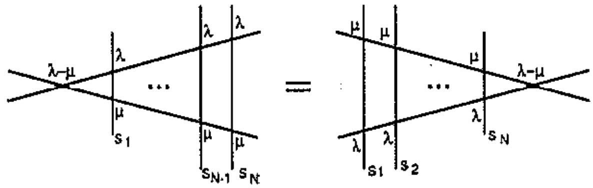

Figure 3. Diagrammatic representation of equation (2.10).

Next we introduce the monodromy matrix $\hat{I}_S(\lambda)$

$$\hat{I}_S(\lambda) = {}_SR^{01}(\lambda)\, {}_SR^{02}(\lambda) \ldots {}_SR^{0m}(\lambda)\, {}_{SS'}R^{0\text{imp}}(\lambda)\, {}_SR^{0m+1}(\lambda) \ldots {}_SR^{0N}(\lambda) \tag{2.6}$$

where the matrix product is carried out in the auxiliary space V_0 of dimension $(2S + 1)$. Note that a vertex weight for the impurity (of spin $S' = \frac{1}{2}$) has been inserted between the sites m and $(m + 1)$. A schematic representation of the monodromy matrix is given in figure 2. The V_0 space is denoted by the horizontal line, all others by vertical lines. Taking the trace over the in- and outgoing V_0 lines (i.e. by forming a ring) we obtain the transfer matrix $T_S(\lambda)$,

$$T_S(\lambda) = \text{Tr}_0(\hat{I}_S(\lambda)). \tag{2.7}$$

As a consequence of the triangular Yang–Baxter relation satisfied by all the vertex weights, the transfer matrices for different values of the parameter λ commute,

$$[T_S(\lambda), T_S(\mu)] = 0. \tag{2.8}$$

Hence, there exists a basis of states that diagonalizes $T_S(\lambda)$ for all λ simultaneously. The Hamiltonian, i.e. the energy associated with the transfer matrix, is then constructed according to

$$H = \frac{\mathrm{d}}{\mathrm{d}\lambda} \ln T_S(\lambda)|_{\lambda=0}. \tag{2.9}$$

In the absence of an impurity this procedure leads to the Babujian–Takhtajan SU(2)-invariant Heisenberg chain of spin S. A special case of the Babujian–Takhtajan model is the standard Heisenberg chain of spin $\frac{1}{2}$. For $S = \frac{1}{2}$ and an arbitrary impurity spin S', the above procedure has been employed by Andrei and Johannesson [24] and for $S = 1$ and arbitrary S' by Lee and Schlottmann [25]. Critical behaviour induced by the impurity, however, only arises for $S > 1$ and $S' < S$. To show this is the main purpose of the paper. For $S = 1$ and $S' = \frac{1}{2}$ the critical behaviour due to the impurity is marginal, i.e. χ and C/T diverge logarithmically as H and T tend to zero.

Next we prove the relation (2.8). Consider the identity

$$ {}_SR(\lambda - \mu)[\hat{I}_S(\lambda) \otimes \hat{I}_S(\mu)] = [\hat{I}_S(\mu) \otimes \hat{I}_S(\lambda)]\, {}_SR(\lambda - \mu) \tag{2.10}$$

which is schematically shown in figure 3. It is clear from this figure that the identity follows straightforwardly from the triangular relation (2.1). Multiplying equation (2.10) by $[{}_SR(\lambda - \mu)]^{-1}$ from the left we obtain

$$\hat{I}_S(\lambda) \otimes \hat{I}_S(\mu) = [{}_SR(\lambda - \mu)]^{-1}[\hat{I}_S(\mu) \otimes \hat{I}_S(\lambda)]\, {}_SR(\lambda - \mu). \tag{2.11}$$

Taking the trace over both auxiliary spaces the left-hand side just yields $T_S(\lambda)T_S(\mu)$. The right-hand side is the trace over a product of operators, which is invariant under a cyclic permutation of these operators. Hence, the right-hand side yields $T_S(\mu)T_S(\lambda)$, proving in this way equation (2.8). An analytic continuation argument can be invoked for those points where $[{}_SR(\lambda-\mu)]^{-1}$ does not exist.

Rather than diagonalizing $T_S(\lambda)$ (which is a $(2S+1)\times(2S+1)$ matrix) for all λ simultaneously, we choose the simple way outlined in [14] and [18]. We introduce a second monodromy matrix, defined over a two-dimensional auxiliary space σ,

$$\hat{J}_\sigma(\lambda) = {}_{\sigma S}R^{01}(\lambda)\ {}_{\sigma S}R^{02}(\lambda)\dots {}_{\sigma S}R^{0m}(\lambda)\ {}_{\sigma S'}R^{0\,\mathrm{imp}}(\lambda)\,{}_{\sigma S}R^{0m+1}(\lambda)\dots {}_{\sigma S}R^{0N}(\lambda) \tag{2.12}$$

so tht $\hat{J}_\sigma(\lambda)$ is now a two-dimensional matrix in V_0. Again an impurity of spin S' is introduced between the sites m and $m+1$. This is a necessary condition to construct the following identity,

$$_{\sigma S}R(\lambda-\mu)[\hat{J}_\sigma(\lambda)\otimes\hat{I}_S(\mu)] = [\hat{I}_S(\mu)\otimes\hat{J}_\sigma(\lambda)]\ {}_{\sigma S}R(\lambda-\mu) \tag{2.13}$$

which follows straightforwardly from the triangular relation (2.1). Proceeding in a similar way as in equation (2.11) we obtain, taking the trace over both auxiliary spaces,

$$[T_\sigma(\lambda), T_S(\mu)] = 0 \tag{2.14}$$

where $T_\sigma(\lambda) = \mathrm{Tr}_0(\hat{J}_\sigma(\lambda))$. Hence, there exists a basis that diagonalizes simultaneously $T_\sigma(\lambda)$ and $T_S(\mu)$ for all λ and μ. Similarly, using the identity

$$_{\sigma}R(\lambda-\mu)[\hat{J}_\sigma(\lambda)\otimes\hat{J}_\sigma(\mu)] = [\hat{J}_\sigma(\mu)\otimes\hat{J}_\sigma(\lambda)]\ {}_{\sigma}R(\lambda-\mu) \tag{2.15}$$

one can show that

$$[T_\sigma(\lambda), T_\sigma(\mu)] = 0. \tag{2.16}$$

Hence, the basis that diagonalizes $T_\sigma(\lambda)$ for all λ also diagonalizes $T_S(\mu)$ for all μ.

$\hat{J}_\sigma(\lambda)$ is a 2×2 matrix in auxiliary space, which can be written as

$$\hat{J}_\sigma(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix} \tag{2.17}$$

where A, B, C and D are operators built from products of vertex weights. The diagonalization of $T_\sigma(\lambda)$ then corresponds to diagonalizing $A(\lambda)+D(\lambda)$. Inserting (2.2) into (2.15) and carrying out the matrix products one arrives at the following commutation relations for the operators A, B, C and D:

$$[A(\lambda), A(\mu)] = [D(\lambda), D(\mu)] = 0 \tag{2.18a}$$

$$[B(\lambda), B(\mu)] = [C(\lambda), C(\mu)] = 0 \tag{2.18b}$$

$$B(\lambda)A(\mu) = [1/(1-\lambda+\mu)]B(\mu)A(\lambda) - [(\lambda-\mu)/(1-\lambda+\mu)]A(\mu)B(\lambda) \tag{2.18c}$$

$$B(\mu)D(\lambda) = [1/(1-\lambda+\mu)]B(\lambda)D(\mu) - [(\lambda-\mu)/(1-\lambda+\mu)]D(\lambda)B(\mu). \tag{2.18d}$$

We denote with Ω_0 the state of maximum spin, i.e. the state in which all spins S in

$\hat{J}_\sigma(\lambda)$ have S_z projection S and the impurity has S_z projection S'. Now ${}_{\sigma S}R^{0n}(\lambda)$ applied on Ω_0 yields (here n is the site index)

$$ {}_{\sigma S}R^{0n}(\lambda)\Omega_0 = \begin{pmatrix} \frac{1}{2}(1-2\lambda)+S & S_n^- \\ 0 & \frac{1}{2}(1-2\lambda)-S \end{pmatrix} \Omega_0. \tag{2.19}$$

If n is the impurity site, then S is to be replaced by S'. It follows immediately that the eigenvalues of $A(\lambda)\Omega_0 = \Lambda_A(\lambda)\Omega_0$ and $D(\lambda)\Omega_0 = \Lambda_D(\lambda)\Omega_0$ are given by

$$\begin{aligned} \Lambda_A(\lambda) &= [\tfrac{1}{2}(1-2\lambda)+S]^N[\tfrac{1}{2}(1-2\lambda)+S'] \\ \Lambda_D(\lambda) &= [\tfrac{1}{2}(1-2\lambda)-S]^N[\tfrac{1}{2}(1-2\lambda)-S'] \end{aligned} \tag{2.20}$$

and that $C(\lambda)\Omega_0 = 0$.

Next we define a state with M flipped spins as

$$\Omega(\lambda_1', \ldots, \lambda_M') = \prod_{l=1}^{M} B(\lambda_l')\Omega_0. \tag{2.21}$$

In view of equation (2.19) we can interpret B as a spin lowering operator. Hence, the sequential application of M operators B yields a state with total spin projection $(NS + S' - M)$. Here $\{\lambda_l'\}$ is a set of M parameters to be determined by the condition that $\Omega(\lambda_1', \ldots, \lambda_M')$ is an eigenstate of $A(\lambda) + D(\lambda)$. After some algebra we obtain

$$\begin{aligned}[][A(\lambda)+D(\lambda)]\Omega(\lambda_1', \ldots, \lambda_M') &= [A(\lambda)+D(\lambda)]\prod_{l=1}^{M} B(\lambda_l')\Omega_0 \\ &= \Lambda(\lambda, \{\lambda_l'\})\prod_{l=1}^{M} B(\lambda_l')\Omega_0 + \sum_{n=1}^{M} \Lambda_n(\lambda, \{\lambda_l'\}) \prod_{\substack{l=1 \\ l\neq n}}^{M} B(\lambda_l')B(\lambda)\Omega_0 \end{aligned} \tag{2.22}$$

where

$$\Lambda(\lambda, \{\lambda_l'\}) = \Lambda_A(\lambda)\prod_{l=1}^{M}\frac{\lambda-\lambda_l'+1}{\lambda-\lambda_l'} + \Lambda_D(\lambda)\prod_{l=1}^{M}\frac{\lambda-\lambda_l'-1}{\lambda-\lambda_l'} \tag{2.23}$$

and

$$\begin{aligned}\Lambda_n(\lambda, \{\lambda_l'\}) = &-\frac{1}{\lambda-\lambda_n'}\Lambda_A(\lambda_n')\prod_{\substack{l=1 \\ l\neq n}}^{M}\frac{\lambda_n'-\lambda_l'+1}{\lambda_n'-\lambda_l'} \\ &+\frac{1}{\lambda-\lambda_n'}\Lambda_D(\lambda_n')\prod_{l=1\, l\neq n}^{M}\frac{\lambda_n'-\lambda_l'-1}{\lambda_n'-\lambda_l'}. \end{aligned} \tag{2.24}$$

Here we have commuted $(A + D)$ through all the B operators by making use of equations (2.18). If the second term on the right-hand side of (2.22) vanishes, then $\Omega(\lambda_1', \ldots, \lambda_M')$ is an eigenvector of $(A + D)$ with eigenvalue given by equation (2.23). This is the case if $\Lambda_n(\lambda, \{\lambda_l'\}) = 0$ for $n = 1, \ldots, M$, so that all the 'unwanted' terms disappear. These M constraints determine the auxiliary parameters λ_l'. Setting

$\lambda_n' = \mathrm{i}\Lambda_n + \frac{1}{2}$ we finally obtain the Bethe *ansatz* equations for the Heisenberg chain with impurity ($S' = \frac{1}{2}$):

$$\left(\frac{\Lambda_n + \mathrm{i}S}{\Lambda_n - \mathrm{i}S}\right)^N \frac{\Lambda_n + \mathrm{i}S'}{\Lambda_n - \mathrm{i}S'} = -\prod_{l=1}^{M} \frac{\Lambda_n - \Lambda_l + \mathrm{i}}{\Lambda_n - \Lambda_l - \mathrm{i}} \tag{2.25}$$

where $n = 1, \ldots, M$. The second factor on the left-hand side of equation (2.25) is due to the impurity.

The Bethe *ansatz* equations (2.25) diagonalize $T_\sigma(\lambda)$ for all λ and, as argued above, simultaneously $T_S(\lambda)$ for all λ. The eigenvalue of $T_\sigma(\lambda)$ is given by equation (2.23). The energy of our system is, however, determined from the eigenvalue of $T_S(\lambda)$ through equation (2.9). To calculate this eigenvalue we would have to consider $\hat{I}_S(\lambda)$, which is a $(2S+1) \times (2S+1)$ dimensional matrix in auxiliary space, and derive the commutation relations corresponding to equations (2.18) for the non-trivial components of $\hat{I}_S(\lambda)$. Following a procedure analogous to equation (2.22) we then obtain the desired eigenvalue. The 'unwanted' terms vanish identically if the set $\{\lambda_l'\}$ satisfies the Bethe *ansatz* equations (2.25).

We are mainly interested in the impurity contribution to the energy. There is an alternative way to obtain this contribution, namely via the self-consistent solutions of equations (2.25) used in the energy expression for the chain without impurity. This procedure has been frequently employed to calculate the energy associated with a magnetic impurity in a metal (Kondo problem). The impurity factor in equations (2.25) then generates the desired energy change (which is a $1/N$ effect). The expression of the energy of the chain without impurity has been obtained previously by Babujian [18] and is given by

$$E = -\sum_{l=1}^{M} [S/(\Lambda_l^2 + S^2)]. \tag{2.26}$$

Finally, we would like to sketch the method to derive the Hamiltonian describing the interaction of the chain with the impurity. This Hamiltonian has been constructed in [24] for $S = \frac{1}{2}$ and arbitrary S' and in [25] for $S = 1$ and arbitrary impurity spin S'. Since the impurity only interacts with the spins at the sites labelled m and $m+1$, it is actually only necessary to consider

$$T^*(\lambda) = \mathrm{Tr}_0({}_S R^{0m}(\lambda)_{SS'} R^{0\,\mathrm{imp}}(\lambda)\, {}_S R^{0m+1}(\lambda)). \tag{2.27}$$

The matrix product and the trace are evaluated in the auxiliary space V_0 of spin S. Now H_{int} is obtained via

$$H_{\mathrm{int}} = H^* - 2H_{m,m+1} \tag{2.28}$$

where

$$H^* = \frac{\mathrm{d}}{\mathrm{d}\lambda} \ln T^*(\lambda)|_{\lambda=0}$$

and $H_{m,m+1}$ is the interaction between the sites m and $m+1$. This subtraction is necessary since the trace in (2.27) links these two sites. Since H^* and $T^*(\lambda)$ commute, they can be diagonalized within the same basis of eigenstates. Since H^* is invariant under the permutation of the sites m and $m+1$, the eigenfunctions should have well defined parity. The total angular momentum $\boldsymbol{J} = \boldsymbol{S}_m + \boldsymbol{S}_{m+1} + \boldsymbol{S}'$ and its z component are good quantum numbers of $T^*(\lambda)$. Owing to the well defined parity it is convenient first to sum $\boldsymbol{S}_m$ and $\boldsymbol{S}_{m+1}$ to give $\boldsymbol{S}^*$, the quantum numbers for S^* being $0, 1, 2, \ldots, 2S$. The Hamiltonian $H_{\rm int}$ is most conveniently expressed as a linear combination of products of irreducible tensor operators for the spins $\boldsymbol{S}_m$, $\boldsymbol{S}_{m+1}$ and $\boldsymbol{S}'$. As a consequence of the rotational invariance and for $S' = \frac{1}{2}$, $H_{\rm int}$ should be of the form

$$H_{\rm int} = P(\boldsymbol{S}_m \cdot \boldsymbol{S}_{m+1}) + [(\boldsymbol{S}' \cdot \boldsymbol{S}_m) + (\boldsymbol{S}' \cdot \boldsymbol{S}_{m+1})]Q(\boldsymbol{S}_m \cdot \boldsymbol{S}_{m+1}) \tag{2.29}$$

where P and Q are polynomials of order $2S$ and $2S-1$, respectively.

Equations (2.25) are also the Bethe *ansatz* equations for an impurity of arbitrary spin S', which are solved in the following section.

3. Thermodynamic equations

The thermodynamic properties of the model are obtained in complete analogy to [6, 18, 25]. Each state of the system corresponds to a solution of the Bethe *ansatz* equations (2.25). In the thermodynamic limit the solutions of equations (2.25) lie in the complex plane and form strings of length n

$$\Lambda_j^{n,\alpha} = \Lambda_j^n + \mathrm{i}(n+1-2\alpha)/2 \qquad \alpha = 1, 2, \ldots, n \tag{3.1}$$

where Λ_j^n is the centre of the string and a real number. The length of the string is in principle arbitrary, $n = 1, 2, \ldots$. Let ξ_n be the number of strings of length n; then we must satisfy

$$M = \sum_{n=1}^{\infty} n\xi_n. \tag{3.2}$$

A string excitation of order n represents a bound-magnon state of n magnons.

Substituting (3.1) into (2.25) we obtain the following relations by taking logarithms:

$$N\Theta_{n,2S}(\Lambda_j^n) + \Theta_{n,2S'}(\Lambda_j^n) = 2\pi J_j^n + \sum_{k=1}^{\infty}\sum_{l=1}^{\xi_k} \Xi_{n,k}(\Lambda_j^n - \Lambda_l^k) \tag{3.3}$$

where

$$\Theta_{n,2S}(\Lambda) = \sum_{l=1}^{\min(n,2S)} 2\arctan[2\Lambda/(n+2S+1-2l)] \tag{3.4}$$

and

$$\Xi_{n,k}(\Lambda) = 2\arctan[2\Lambda/(n+k)] + 4\sum_{l=1}^{\min(k,n)-1} \arctan[2\Lambda/(n+k-2l)]$$
$$+ \delta_{k\neq n} 2\arctan[2\Lambda/|(n-k)|]. \tag{3.5}$$

In the thermodynamic limit the variable $2\pi J_j^n/N$ becomes closely spaced and can be regarded as continuous. It is then convenient to introduce density functions for each set of rapidities, one for the 'particles' and one for the 'holes'. We denote them by $\rho_n(\Lambda)$ and

$\rho_{n,\mathrm{h}}(\Lambda)$, respectively, where the sub-index n refers to the string length. Differentiating equations (3.3) with respect to Λ_j^n we obtain in the thermodynamic limit

$$\frac{1}{\pi}\sum_{l=1}^{\min(n,2S)}\frac{\frac{1}{2}(n+2S+1-2l)}{\Lambda^2+\frac{1}{4}(n+2S+1-2l)^2}+\frac{1}{N\pi}\sum_{l=1}^{\min(n,2S')}\frac{\frac{1}{2}(n+2S'+1-2l)}{\Lambda^2+\frac{1}{4}(n+2S'+1-2l)^2}$$

$$=\rho_n(\Lambda)+\rho_{n,\mathrm{h}}(\Lambda)+\sum_{k=l}^{\infty}\int \mathrm{d}\Lambda'[A_{n,k}(\Lambda-\Lambda')-\delta_{n,k}\delta(\Lambda-\Lambda')]\rho_k(\Lambda')$$

$$=\rho_{n,\mathrm{h}}(\Lambda)+\sum_{k=1}^{\infty}\mathrm{d}\Lambda'\,A_{n,k}(\Lambda-\Lambda')\rho_k(\Lambda') \tag{3.6}$$

for $n = 1, 2, \ldots$ and where

$$A_{n,k}(\Lambda)=\frac{1}{\pi}\frac{\frac{1}{2}(n+k)}{\Lambda^2+\frac{1}{4}(n+k)^2}+\frac{2}{\pi}\sum_{l=1}^{\min(k,n)-1}\frac{\frac{1}{2}(n+k-2l)}{\Lambda^2+\frac{1}{4}(n+k-2l)^2}+\frac{1}{\pi}\frac{\frac{1}{2}|n-k|}{\Lambda^2+\frac{1}{4}(n-k)^2}. \tag{3.7}$$

The last term in (3.7) is to be interpreted as a δ-function if $k = n$.

The magnetization, $S_z = NS + S' - M$, and the energy, equation (2.26), are given by

$$S_z/N = S + S'/N - \sum_{n=1}^{\infty} n\int \mathrm{d}\Lambda\,\rho_n(\Lambda) \tag{3.8}$$

$$E/N = -\sum_{n=1}^{\infty}\int \mathrm{d}\Lambda\,\rho_n(\Lambda)\sum_{l=0}^{\min(2S,n)}\frac{\frac{1}{2}(n+2S+1-2l)}{\Lambda^2+\frac{1}{4}(n+2S+1-2l)^2}. \tag{3.9}$$

The entropy is given by the distribution of particles and holes, which are exclusive and hence governed by Fermi statistics. We introduce an entropy functional for each class of excitations, so that

$$S/N = \sum_{n=1}^{\infty}\mathrm{d}\Lambda\,[(\rho_n+\rho_{n,h})\ln(\rho_{n,\mathrm{h}})-\rho_n\ln\rho_n-\rho_{n,\mathrm{h}}\ln\rho_{n,\mathrm{h}}]. \tag{3.10}$$

To obtain the free energy we have to impose thermal equilibrium and minimize the functional $F = E - TS$ with respect to the density functions, ρ_n and $\rho_{n,\mathrm{h}}$ for all n, subject to the constraints (3.6) and (3.8). The constraint (3.8) is introduced via a Lagrange multiplier, which is physically interpreted as the magnetic field. The variations $\delta\rho_{n,\mathrm{h}}(\Lambda)$ can be eliminated using (3.6). Introducing an energy potential for each class of excitations

$$\varepsilon_n(\Lambda) = T\ln(\rho_{n,\mathrm{h}}/\rho_n) \tag{3.11}$$

we obtain after some algebra

$$T\ln[1+\exp(\varepsilon_n/T)] = nH - \sum_{l=1}^{\min(2S,n)}\frac{\frac{1}{2}(2S+n+1-2l)}{\Lambda^2+\frac{1}{4}(2S+n+1-2l)^2}$$

$$+T\sum_{k=1}^{\infty}\int \mathrm{d}\Lambda'\,A_{n,k}(\Lambda-\Lambda')\ln[1+\exp(-\varepsilon_k(\Lambda')/T)]. \tag{3.12}$$

Equations (3.12) are the thermodynamic Bethe *ansatz* equations. This infinite set of non-linear integral equations can be expressed in various equivalent ways. In Fourier space these equations become algebraic. The Fourier transform of $A_{n,k}(\Lambda)$ is

$$\hat{A}_{n,k}(\omega) = \coth(|\omega|/2)\{\exp[-|\omega|\,|(k-n)|/2] - \exp[-|\omega|(n+k)/2]\} \tag{3.13}$$

and its inverse is

$$\hat{A}^{-1}_{n,k}(\omega) = \delta_{n,k} - (\delta_{n,k+1} + \delta_{n,k-1})/[2\cosh(\omega/2)]. \tag{3.14}$$

Multiplying the Fourier transform of equation (3.12) by $\hat{A}_{n,m}(\omega)$, summing over n and Fourier transforming back to Λ space one obtains

$$\varepsilon_m(\Lambda) = T\int \mathrm{d}\Lambda'\,\{2\cosh[\pi(\Lambda-\Lambda')]\}^{-1}\ln\{[1+\exp(\varepsilon_{m+1}/T)] \times [1+\exp(\varepsilon_{m-1}/T)]\} - 2\pi\delta_{m,2S}/[2\cosh(\pi\Lambda)]. \tag{3.15}$$

Equations (3.15) are only complete with the asymptotic field boundary condition

$$\lim_{m\to\infty}[\varepsilon_m(\Lambda)/m] = H \tag{3.16}$$

which follows from equations (3.12).

Inserting the thermal equilibrium density functions into the free energy functional we obtain after some algebra the free energy expressions for the host chain and the impurity

$$F_{\mathrm{host}}(H,T) = F^0_{\mathrm{host}} - T\int \mathrm{d}\Lambda\,[2\cosh(\pi\Lambda)]^{-1}\ln[1+\exp(\varepsilon_{2S}/T)] \tag{3.17}$$

$$F_{\mathrm{imp}}(H,T) = F^0_{\mathrm{imp}} - T\int \mathrm{d}\Lambda\,[2\cosh(\pi\Lambda)]^{-1}\ln[1+\exp(\varepsilon_{2S'}/T)] \tag{3.18}$$

where F^0_{host} and F^0_{imp} are constants given by

$$F^0_{\mathrm{host}} = \tfrac{1}{2}[\psi(\tfrac{1}{2}) - \psi(\tfrac{1}{2}+S)] \tag{3.19}$$

$$F^0_{\mathrm{imp}} = \tfrac{1}{2}[\psi(\tfrac{1}{2}+\tfrac{1}{2}|S-S'|) - \psi(\tfrac{1}{2}+\tfrac{1}{2}(S+S'))] \tag{3.20}$$

with ψ being the digamma function.

The solution of equations (3.12) and the thermodynamic properties of the system for small fields and low temperatures are discussed in the following section.

4. Small-field and low-temperature properties of the system

In this section we analyse first the zero-temperature properties of the system in a magnetic field and then the low-temperature behaviour in zero field.

4.1. *Zero-temperature zero-field solution*

Consider equations (3.15) for $T\to 0$. Since for $m \neq 2S$ the right-hand side is always positive, it follows that $\varepsilon_m(\Lambda)$ is positive for $m \neq 2S$ and all Λ. Hence, according to (3.11) the particle states for $m \neq 2S$ are not occupied. This conclusion is valid for all fields in the $T\to 0$ limit. The ground-state properties are then determined by strings of length $2S$, i.e. $2S$ spin waves are glued together (form a bound state) and behave as a unit.

Consider now equation (3.6) for $n = 2S$ and $\rho_k \equiv 0$ for $k \neq 2S$. In Fourier space we obtain

$$\hat{\rho}_{2S,h}(\omega) + \coth(|\omega|/2)[1 - \exp(-2S|\omega|)]\hat{\rho}_{2S}(\omega) = \exp(-S|\omega|)\frac{\sinh(S\omega)}{\sinh(\frac{1}{2}\omega)} + \frac{1}{N}\exp[-\max(S,S')|\omega|]\frac{\sinh[\min(S,S')\omega]}{\sinh(\frac{1}{2}\omega)}. \tag{4.1}$$

The zero-field limit is characterized by the absence of string holes of length $2S$, i.e. $\rho_{2S,h} \equiv 0$. It follows that

$$\hat{\rho}_{2S}(\omega) = [2\cosh(\omega/2)]^{-1}\left(1 + \frac{1}{N}\exp\{[S - \max(S,S')]|\omega|\}\frac{\sinh[\min(S,S')\omega]}{\sinh(S\omega)}\right) \tag{4.2}$$

and using equation (3.9) we arrive at

$$E = -\tfrac{1}{2}\int d\omega\, \hat{\rho}_{2S}(\omega)\, e^{-S|\omega|}[\sinh(S\omega)/\sinh(\tfrac{1}{2}\omega)]. \tag{4.3}$$

Inserting (4.2) into (4.3) we obtain the zero-field ground-state energy, $E = F^0_{\text{host}} + N^{-1}F^0_{\text{imp}}$, where F^0_{host} and F^0_{imp} are defined by equations (3.19) and (3.20).

4.2. Zero-temperature solution in a finite field

We now consider equations (3.12) in the limit $T \to 0$. Defining as ε_n^+ the positive part of ε_n and as ε_n^- its negative part, we have after Fourier transformation

$$\hat{\varepsilon}_n^+(\omega) = 2\pi n H\delta(\omega) - \pi\hat{A}_{2S,n}(\omega)[2\cosh(\omega/2)]^{-1} - \hat{A}_{2S,n}(\omega)\hat{\varepsilon}_{2S}^-(\omega) \tag{4.4}$$

since ε_{2S} is the only potential with a negative part. Consider first the zero-field limit of (4.4) for $n = 2S$. Since $\varepsilon_{2S}^+ \equiv 0$ if $H = 0$, it follows that

$$\varepsilon_{2S}(\Lambda) = -\tfrac{1}{2}\pi/\cosh(\pi\Lambda) \tag{4.5}$$

and for $n \neq 2S$ we have $\varepsilon_n = 0$.

From (3.18) the $T \to 0$ impurity free energy limit is

$$F^{S'}_{\text{imp}}(T=0,H) = F^0_{\text{imp}} - \int \frac{d\omega}{2\pi}[2\cosh(\omega/2)]^{-1}\hat{\varepsilon}_{2S'}^+(\omega) \tag{4.6}$$

which in the limit $H = 0$ agrees with the result (4.3), since $\hat{\varepsilon}_{2S'}^+(\omega) \equiv 0$. Using equation (4.4) for $n = 2S'$ and $n = 2S$ we express the impurity ground-state energy in an arbitrary field as

$$F^{S'}_{\text{imp}}(T=0,H) = F^0_{\text{imp}} - [S' - \min(S,S')]H - \int \frac{d\omega}{2\pi}[2\cosh(\omega/2)]^{-1} \times \{\exp[-|\omega|\,|(S-S')|] - \exp[-|\omega|(S+S')]\}/[1 - \exp(-2S|\omega|)]\hat{\varepsilon}_{2S}^+(\omega) \tag{4.7}$$

where (3.13) has been used. The supra-index S' in $F^{S'}_{\text{imp}}$ is to indicate that it refers to an impurity spin S'. In other words, by solving the integral equation (4.4) for $n = 2S$, we are able to obtain the free energy for arbitrary impurity spin via (4.7).

The function $\varepsilon_{2S}(\Lambda)$ is symmetric in Λ, negative for small Λ, grows monotonically with $\Lambda > 0$ and is positive (if $H \neq 0$) as $\Lambda \to \infty$. Hence, ε_{2S} has zeros at $\varepsilon_{2S}(\pm B) = 0$, where B is a function of H, tending to ∞ as $H \to 0$.

Following the procedure described in [18] we solve equation (4.4) for $n = 2S$ iteratively for small fields as a sequence of Wiener–Hopf integral equations. Dividing equation (4.4) by $\hat{A}_{2S,2S}(\omega)$ we have

$$\varepsilon_{2S}(\Lambda) = \tfrac{1}{2}H - \tfrac{1}{2}\pi/\cosh(\pi\Lambda) + \left(\int_{-\infty}^{-B} + \int_{B}^{\infty}\right) \mathrm{d}\Lambda'\, J(\Lambda - \Lambda')\varepsilon_{2S}(\Lambda') \tag{4.8}$$

where

$$J(\Lambda) = \int \frac{\mathrm{d}\omega}{2\pi} \mathrm{e}^{-\mathrm{i}\Lambda\omega}\{1 - [\hat{A}_{2S,2S}(\omega)]^{-1}\}. \tag{4.9}$$

We now define $y(\Lambda) = \varepsilon_{2S}(\Lambda + B)$, so that $y(\Lambda = 0)$ corresponds to the 'Fermi surface' of strings of length $2S$ (no other states have a Fermi surface). In terms of $y(\Lambda)$ equation (4.8) reads

$$y(\Lambda) = \tfrac{1}{2}H - \tfrac{1}{2}\pi/\cosh[\pi(\Lambda + B)] + \int_0^{\infty} \mathrm{d}\Lambda'\, J(\Lambda - \Lambda')y(\Lambda') + \int_0^{\infty} \mathrm{d}\Lambda'\, J(\Lambda + \Lambda' + 2B)y(\Lambda') \tag{4.10}$$

where we have used that $\varepsilon_{2S}(\Lambda) = \varepsilon_{2S}(-\Lambda)$. If $H \ll 1$, B is very large and $J(\Lambda + \Lambda' + 2B) \sim 1/B$, so that the last term is order $1/B$ smaller than the previous ones. Writing $y(\Lambda) = y_1(\Lambda) + y_2(\Lambda) + \ldots$, we solve equation (4.10) iteratively with $y_1(\Lambda)$ and $y_2(\Lambda)$ satisfying

$$y_1(\Lambda) = \tfrac{1}{2}H - \tfrac{1}{2}\pi/\cosh[\pi(\Lambda + \mathrm{B})] + \int_0^{\infty} \mathrm{d}\Lambda'\, J(\Lambda - \Lambda')y_1(\Lambda') \tag{4.11}$$

$$y_2(\Lambda) = \int_0^{\infty} \mathrm{d}\Lambda'\, J(\Lambda - \Lambda')y_2(\Lambda') + \int_0^{\infty} \mathrm{d}\Lambda'\, J(\Lambda + \Lambda' + 2B)y_1(\Lambda') \tag{4.12}$$

etc. These equations are of the Wiener–Hopf type and can be solved analytically.

Denoting with y^+ and y^- the positive ($\Lambda > 0$) and negative ($\Lambda < 0$) parts of y we obtain on Fourier transforming equation (4.11)

$$\hat{y}_1^+(\omega)/\hat{A}_{2S,2S}(\omega) + \hat{y}_1^-(\omega) = \pi H\delta(\omega) - \tfrac{1}{2}\pi\, \mathrm{e}^{-\mathrm{i}\omega B}/\cosh(\omega/2). \tag{4.13}$$

In order to apply the Wiener–Hopf method $[\hat{A}_{2S,2S}(\omega)]^{-1}$ has to be written as a product of two functions, one $G_{2S}^+(\omega)$, analytic in the upper half-plane, the other, $G_{2S}^-(\omega)$, analytic in the lower half-plane,

$$G_{2S}^+(\omega) = G_{2S}^-(-\omega) = \frac{1}{2(S\pi)^{1/2}}\left(\frac{-\mathrm{i}\omega + 0}{a}\right)^{\mathrm{i}S\omega/\pi} \frac{\Gamma(\frac{1}{2} - \mathrm{i}\omega/2\pi)\Gamma(1 - \mathrm{i}S\omega/\pi)}{\Gamma(1 - \mathrm{i}\omega/2\pi)}. \tag{4.14}$$

The constant $a = \pi\mathrm{e}/S$ is determined so that $G_{2S}^{\mp}(\infty)$ is constant. From the analytic properties of the functions $\hat{y}_1^{\mp}(\omega)$ and $G_{2S}^{\mp}(\omega)$ it follows that

$$\hat{y}_1^+(\omega) = -q_+(\omega)/G_{2S}^+(\omega) \qquad \hat{y}_1^-(\omega) = +q_-(\omega)G_{2S}^-(\omega) \tag{4.15}$$

where

$$q_\pm(\omega) = -\mathrm{i}S^{1/2}H/(\omega \pm \mathrm{i}0) - \tfrac{1}{2}\mathrm{i}\int \frac{\mathrm{d}\omega'}{2\pi} \frac{\Gamma(\frac{1}{2} + \mathrm{i}\omega'/2\pi)\Gamma(\frac{1}{2} - \mathrm{i}\omega'/2\pi)}{\omega' - \omega \mp \mathrm{i}0} \frac{\mathrm{e}^{-\mathrm{i}\omega' B}}{G_{2S}^-(\omega')}. \tag{4.16}$$

We are actually interested in $\hat{y}_1^+(\omega)$ for large B, so that the contour integral (4.16) can be closed through the lower half-plane. The value of the integral is given by the sum of the residua of $\Gamma(\frac{1}{2} - i\omega'/2\pi)$. Keeping only the leading term (the pole closest to the real axis) we obtain

$$\hat{y}_1^+(\omega) = \frac{iS^{1/2}}{G_{2S}^+(\omega)}\left[\frac{H}{\omega + i0} - \frac{\pi^2}{\Gamma(1+S)}\left(\frac{S}{e}\right)^S \frac{e^{-\pi B}}{\omega + i\pi}\right]. \tag{4.17}$$

Note that next-order corrections are of the order $e^{-2\pi B}$ smaller.

Corrections due to y_2 are only of the order $1/B$ smaller and should not be neglected in general. The Fourier transform of equation (4.12) can be written as

$$\hat{y}_2^+(\omega)G_{2S}^+(\omega) + \hat{y}_2^-(\omega)/G_{2S}^-(\omega) = [1/G_{2S}^-(\omega) - G_{2S}^+(\omega)]\, e^{-2i\omega B}\hat{y}_1^+(-\omega) \tag{4.18}$$

where $\hat{y}_1^+(-\omega)$ is analytic in the lower half-plane. Again, from the analytic properties of $y^\pm$ and $G^\pm$ it follows that

$$\hat{y}_2^+(\omega)G_{2S}^+(\omega) = (-i/2\pi)\int d\omega'\, e^{-2i\omega' B}[\hat{y}_1^+(-\omega')/(\omega' - \omega - i0)]$$
$$\times [1/G_{2S}^-(\omega') - G_{2S}^+(\omega')]. \tag{4.19}$$

Since B is large and positive, we close the contour through the lower half-plane; here only $G^+(\omega')$ has singularities, the leading one being the cut along the imaginary axis. For our next step, which is the determination of $B(H)$, we only need $y_2^+(\omega \to \infty)$, which is of the order H/B.

The parameter B is a function of H and is determined from the condition that $y(\Lambda = 0) = 0$ or $\varepsilon_{2S}(B) = 0$. In Fourier space this condition is equivalent to $\lim_{\omega\to\infty} \omega\hat{y}^+(\omega) = 0$ and using (4.17) and (4.19) we obtain

$$H\left\{1 + \tfrac{1}{2}\left(\frac{S}{\pi B}\right) + \tfrac{1}{4}\left(\frac{S}{\pi B}\right)^2 \ln\left(\frac{S}{\pi B}\right) + \ldots\right\} = [\pi^2/\Gamma(1+S)](S/e)^S\, e^{-\pi B}. \tag{4.20}$$

We are now prepared to calculate the $T = 0$ impurity free energy for the three situations (i) $S' = S$, (ii) $S' > S$ and (iii) $S' < S$ in the limit of small fields. Note that since $\varepsilon_{2S}^+(\Lambda + B) = y^+(\Lambda)$, we have $\hat{\varepsilon}_{2S}^+(\omega) = e^{i\omega B}\hat{y}^+(\omega)$. We use this relation in equation (4.7).

4.2.1. $S' = S$. In this case the impurity is just one more site in the chain and $F_{\mathrm{imp}} = F_{\mathrm{host}}/N$. Equation (4.7) reduces to

$$F_{\mathrm{imp}}^S(T=0, H) = \tfrac{1}{2}[\psi(\tfrac{1}{2}) - \psi(\tfrac{1}{2} + S)] - \int \frac{d\omega}{2\pi}\frac{e^{i\omega B}\hat{y}^+(\omega)}{2\cosh(\omega/2)} \tag{4.21}$$

where the contour is to be closed through the upper half-plane and the value of the integral is given by the residua of the poles of $[\cosh(\omega/2)]^{-1}$. The leading order contribution arises from the pole closest to the real axis, $\omega = i\pi$, and is $-e^{-\pi B}\hat{y}^+(i\pi)$. This term is of the order of H^2; in general the pole at $\omega = i(2n+1)\pi$, $n \geqslant 0$, yields a term of the order H^{2n+2}. $\hat{y}_1^+(i\pi)$ is given by (4.17) and $\hat{y}_2^+(i\pi)$ can be obtained from (4.19)

$$\hat{y}_2^+(i\pi) = [S^2H/2\pi\Gamma(1+S)](S/e)^S[1/B + (S/\pi B^2)\ln(S/2\pi e B)] \tag{4.22}$$

so that

$$F_{\mathrm{imp}}^S(T=0, H) = \tfrac{1}{2}[\psi(\tfrac{1}{2}) - \psi(\tfrac{1}{2} + S)] - (SH^2/2\pi^2)[1 + S/|\ln H|$$
$$- S^2(\ln|\ln H|)/(\ln H)^2 + \ldots]. \tag{4.23}$$

Equation (4.23) is in agreement with Babujian's results and shows the existence of logarithmic singularities in the small-field susceptibility.

4.2.2. $S' > S$. In this case the impurity spin is expected to be partially compensated by the antiferromagnetic chain. The impurity free energy reduces to

$$F^{S'}_{\mathrm{imp}}(T=0,H) = \tfrac{1}{2}[\psi(\tfrac{1}{2}+\tfrac{1}{2}(S'-S)) - \psi(\tfrac{1}{2}+\tfrac{1}{2}(S'+S))] - (S'-S)H - \int \frac{\mathrm{d}\omega}{2\pi}\frac{\exp[\mathrm{i}\omega B - (S'-S)|\omega|]\hat{y}^{+}(\omega)}{2\cosh(\omega/2)} \tag{4.24}$$

where the contour of the integral is to be closed through the upper half-plane. The value of the integral is given by the residua of the poles of $[\cosh(\omega/2)]^{-1}$ and the cut of $\exp[-(S'-S)|\omega|]$ along the imaginary axis. The leading contribution originates from the cut, which is more conveniently analysed by writing

$$\exp[-(S'-S)|\omega|] = [(-\mathrm{i}\omega+0)/(+\mathrm{i}\omega+0)]^{-\mathrm{i}\omega(S'-S)/\pi}. \tag{4.25}$$

The cut gives rise to free energy terms proportional to the field, while the poles, as in (4.23), give rise to contributions of the order of H^{2n+2}, $n = 0, 1, 2, \ldots$. After some calculations we obtain

$$F^{S'}_{\mathrm{imp}}(T=0,H) = \tfrac{1}{2}[\psi(\tfrac{1}{2}+\tfrac{1}{2}(S'-S)) - \psi(\tfrac{1}{2}+\tfrac{1}{2}(S'+S))] - (S'-S)H[1 + S/|\ln H| - S^2(\ln|\ln H|)/(\ln H)^2 + \ldots]. \tag{4.26}$$

This result shows that at $T = 0$ the impurity has an effective spin $(S' - S)$ that is weakly coupled to the spins in the chain. This weak coupling manifests itself in the logarithmic corrections in equation (4.26). Note that we only used $\hat{y}^{+}_{1}(\omega)$ in (4.24), since $\hat{y}^{+}_{2}(\omega)$ gives rise to contributions of the order of $H/(\ln H)^2$ and higher.

4.2.3. $S' < S$. In this case the impurity spin is smaller than the lattice spins and their collective behaviour leads to critical properties. From equation (4.7) the impurity free energy is given by

$$F^{S'}_{\mathrm{imp}}(T=0,H) = \tfrac{1}{2}[\psi(\tfrac{1}{2}+\tfrac{1}{2}(S-S')) - \psi(\tfrac{1}{2}+\tfrac{1}{2}(S+S'))] - \int \frac{\mathrm{d}\omega}{2\pi}\frac{\mathrm{e}^{\mathrm{i}\omega B}\hat{y}^{+}(\omega)\sinh(S'\omega)}{2\cosh(\omega/2)\sinh(S\omega)} \tag{4.27}$$

where, again, the contour integral is to be closed through the upper half-plane. There are poles arising from the zeros of $\cosh(\omega/2)$ and $\sinh(S\omega)$. The leading contribution is due to the pole at $\mathrm{i}\pi/S$, which yields $H^{1/S}$ when inserted into $\mathrm{e}^{\mathrm{i}\omega B}$. Since for small fields $\hat{y}^{+}_{1}$ is proportional to H we obtain

$$F^{S'}_{\mathrm{imp}}(T=0,H) = \tfrac{1}{2}[\psi(\tfrac{1}{2}+\tfrac{1}{2}(S-S')) - \psi(\tfrac{1}{2}+\tfrac{1}{2}(S+S'))] - AH^{1+1/S} \tag{4.28}$$

where the constant A is given by

$$A = \left(\frac{\mathrm{e}}{\pi}\right)^{1/2}\frac{\sin(\pi S'/S)}{\cos(\pi/2S)}\frac{\Gamma(1+1/(2S))}{\Gamma(\tfrac{1}{2}+1/(2S))}\frac{[\Gamma(1+S)]^{1/S}}{\pi^{2/S}(1+S)}.$$

Contributions arising from $\hat{y}^{+}_{2}$ are of the order $H^{1+1/S}/\ln H$, i.e. they yield logarithmic corrections to the critical behaviour. The exponent of the next-to-leading term in (4.28) is $(1 + 2/S)$.

The above arguments are not valid if $S = 1$ (and $S' = \frac{1}{2}$), where the field-dependent term in (4.28) would be just H^2 and hence regular. This is not the case, since in (4.27) the single pole at $\mathrm{i}\pi/S$ for $S > 1$ is a second-order pole if $S = 1$, since both $\cosh(\omega/2)$ and $\sinh(\omega)$ have zeros. The leading field-dependent term is then $-(2/\pi^3)H^2|\ln H|$.

As a consequence of the field-dependent term in (4.28) 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. For $S = 1$ (and hence $S' = \frac{1}{2}$) the exponent vanishes, and a logarithmic divergence emerges.

4.3. Zero-field solution at low temperatures

We now consider equation (3.15) for low temperatures, i.e. $T \ll 1$. Following a similar procedure as for the n-channel Kondo problem [30] we introduce a shift in the rapidity parameter, $\Lambda = \lambda - (1/\pi)\ln(T/2\pi)$, and define

$$\varphi_m(\lambda) = (1/T)\varepsilon_m[\lambda - (1/\pi)\ln(T/2\pi)] = (1/T)\varepsilon_m(\Lambda). \tag{4.29}$$

In terms of the φ_m, equations (3.15) take the form

$$\varphi_m(\lambda) = \int \mathrm{d}\lambda' \, \{2\cosh[\pi(\lambda-\lambda')]\}^{-1} \ln\{[1+\exp(\varphi_{m+1}(\lambda'))] \times [1+\exp(\varphi_{m-1}(\lambda'))]\} - \delta_{m,2S}\exp(-\pi\lambda) \tag{4.30}$$

so that the temperature has formally disappeared as a parameter. The asymptotic field boundary condition for φ_m is

$$\lim_{m\to\infty} \varphi_m(\lambda) = nH/T \tag{4.31}$$

which follows from equation (3.16). In the limits $\varphi \to \pm\infty$ equations (4.30) reduce to algebraic ones and can straightforwardly be solved [31]

$$1+\exp[\varphi_m(\lambda\to\infty)] = \{\sinh[(m+1)H/2T]/\sinh(H/2T)\}^2 \qquad \forall m \tag{4.32}$$

$$1+\exp[\varphi_m(\lambda\to-\infty)] = \begin{cases} \{\sin[(m+1)\pi/(2S+2)]/\sin[\pi/(2S+2)]\}^2 & m \leqslant 2S \\ \{\sinh[(m+1-2S)H/2T]/\sinh(H/2T)\}^2 & m \geqslant 2S. \end{cases} \tag{4.33}$$

We now use this solution in the free energy, which according to equation (3.18) can be written as

$$F_{\mathrm{imp}}(H,T) = F^0_{\mathrm{imp}} - T\int \mathrm{d}\lambda \ln\{1+\exp[\varphi_{2S'}(\lambda)]\}/\{2\cosh[\pi\lambda - \ln(T/2\pi)]\}. \tag{4.34}$$

the 1/cosh function only contributes significantly around $\lambda \sim \ln(T/2\pi) \ll 0$. Inserting equation (4.33) as the solution for $T \to 0$ we obtain $F_{\mathrm{imp}}(H,T) = F_{\mathrm{imp}}(H, T=0) - TS(H, T=0)$

$$\begin{aligned} &\text{(i) } S' = S \quad S(H, T=0) = 0 \\ &\text{(ii) } S' > S \quad S(H=0, T=0) = \ln[2(S'-S)+1] \\ &\qquad\qquad\; S(H\neq 0, T=0) = 0 \\ &\text{(iii) } S' < S \quad S(H=0, T=0) = \ln\{\sin[\pi(2S'+1)/(2S+2)]/\sin[\pi/(2S+2)]\} \\ &\qquad\qquad\; S(H\neq 0, T=0) = 0. \end{aligned} \tag{4.35}$$

The entropy for $S' < S$ in the presence of a field does not follow straightforwardly from

(4.33), but requires further elaboration along the lines of [30, 33]. In summary, we obtained that the zero-field ground state is a singlet only if $S' = S$. Any degeneracy is removed even by a small field, so that the entropy is essentially singular at $H = T = 0$ if $S' \neq S$. This is in agreement with results obtained in section 4.2.

Hence, if $S' = S$ the low-temperature and small-field dependence is Fermi-liquid-like; if $S' > S$ the remaining spin degeneracy of $(S' - S)$ gives rise to a Schottky anomaly for $H \sim T$; and finally if $S' < S$ the effective zero-field degeneracy at $T = 0$ is not an integer, so that non-trivial thermal fluctuations are to be expected. Indeed, critical behaviour is obtained as shown below.

The next step consists in obtaining the next leading order of the temperature dependence for the situation $S' < S$ in zero field. Following [30] we define

$$\begin{aligned} g_m(\lambda) &= \ln\{1 + \exp[\varphi_m(\lambda)]\} \\ \delta g_m(\lambda) &= g_m(\lambda) - g_m(\lambda = -\infty). \end{aligned} \tag{4.36}$$

Assuming that δg_m is small we can linearize equations (4.30) in δg_m and obtain

$$\delta g_m(\lambda)(f_m^2/f_{m+1}f_{m-1}) = \int \mathrm{d}\lambda' \{2\cosh[\pi(\lambda - \lambda')]\}^{-1}[\delta g_{m+1}(\lambda') + \delta g_{m-1}(\lambda')] \tag{4.37}$$

where $f_m^2 = g_m(\lambda = -\infty)$, $f_0 = 1$. We now express $\delta g_m(\lambda)$ for $m < 2S$ in terms of $\delta g_{2S}(\lambda) = g_{2S}(\lambda)$. After some algebra [30, 31, 33] one arrives at (in Fourier space)

$$\delta\hat{g}_m(\omega) = \hat{t}_{m,2S}(\omega)\hat{g}_{2S}(\omega) \tag{4.38}$$

where $\hat{t}_{m,2S}$ is defined as

$$\hat{t}_{j,2S}(\omega) = \frac{f(j-1)\sinh[(j+2)(\omega/2)] - f(j+2)\sinh(j\omega/2)}{2f(j)\cos[\pi/(S+2)]\sinh[(S+1)\omega]}. \tag{4.39}$$

The zero-field free energy is now obtained from (4.34)

$$\begin{aligned} F_{\mathrm{imp}}(H = 0, T) = F^0_{\mathrm{imp}} &- T\ln\{\sin[\pi(2S' + 1)/(2S + 2)]/\sin[\pi/(2S + 2)]\} \\ &- T\int \frac{\mathrm{d}\omega}{2\pi}\, \mathrm{e}^{-\mathrm{i}\omega\ln(T/2\pi)/\pi}[2\cosh(\omega/2)]^{-1}\hat{t}_{2S',2S}(\omega)\hat{g}_{2S}(\omega) \qquad S' < S. \end{aligned} \tag{4.40}$$

The contour of the integral has to be closed through the upper half-plane. The leading contribution arises from the pole at $\omega = 4\pi\mathrm{i}/(2S + 2)$ (the residuum of the pole at $\omega = 2\pi\mathrm{i}/(2S + 2)$ vanishes identically) and is proportional to

$$T^{1+4/(2S+2)}. \tag{4.41}$$

Hence, the specific heat at very low T is proportional to

$$C \sim T^{4/(2S+2)}. \tag{4.42}$$

This result does not hold for $S = 1$ (and $S' = \frac{1}{2}$), where the pole at $\omega = \mathrm{i}\pi$ turns out to be a second-order one and

$$C \sim T\ln(\pi/T) \qquad S = 1, S' = \tfrac{1}{2}. \tag{4.43}$$

In order to obtain the zero-field susceptibility at low T for $S' < S$, we follow a similar procedure [31], now collecting the terms proportional to H^2 (assuming $H \ll T$). A set of integral equations similar to (4.37) is obtained if one linearizes in the field dependence (H^2 terms). After a similar algebra as in the zero-field case

$$\chi \sim T^{-1+4/(2S+2)} \qquad S > 1 \tag{4.44}$$

$$\chi \sim \ln(\pi/T) \qquad S = 1, S' = \tfrac{1}{2}. \tag{4.45}$$

5. Conclusions

Using SU(2)-invariant vertex weights we constructed an integrable variant of the Heisenberg chain of spin S containing one impurity of spin $S' = \frac{1}{2}$ on the mth link interacting with spins at the neighbouring sites. The condition of integrability yields the discrete Bethe *ansatz* equations for the system, from which the thermodynamic properties for arbitrary S and S' have been derived. This extends previous results [24, 25] for $S = \frac{1}{2}$ and $S = 1$ with arbitrary impurity spins S'.

The properties of the system are closely related to those of the generalized n-channel Kondo problem with an impurity spin S'. The thermodynamic Bethe *ansatz* equations are indeed identical at low T for small fields if n equals the spin of the chain, i.e. $n = 2S$. Three situations have to be distinguished. (i) If $S' = S$ the impurity is just one more site in the chain and its properties are identical to those of the 'bulk'. (ii) If $S' > S$ the spins neighbouring the impurity are not able to compensate the impurity spin S' into a singlet at low T and an effective spin $(S' - S)$ remains. A small magnetic field orients this effective spin, which is weakly coupled to the antiferromagnetic chain (Kondo-like logarithmic corrections). The susceptibility diverges as $T \to 0$ for $H = 0$ and the specific heat shows a Schottky anomaly as a function of H/T. (iii) If $S' < S$ again a complete compensation of the impurity spin by the neighbouring lattice sites cannot take place. The impurity is said to be overcompensated. The fixed point in this case has different properties and leads to critical behaviour. The susceptibility diverges as H and T tend to zero,

$$\chi(T = 0, H) \propto H^{-1+1/S} \qquad \chi(T, H = 0) \propto T^{-1+4/(2S+2)} \tag{5.1}$$

and the specific heat over temperature is

$$C(T, H = 0)/T \propto T^{-1+4/(2S+2)} \tag{5.2}$$

Since the field and the temperature have different scaling dimensions, i.e. $1/S$ and $4/(2S + 2)$, respectively, the limits $T \to 0$ and $H \to 0$ cannot be interchanged. For the particular case $S = 1$ and $S' = \frac{1}{2}$ the critical exponents vanish and give rise to logarithmic divergences.

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References

[1] Bethe H A 1931 *Z. Phys.* **71** 205
[2] Hulthén L 1938 *Ark. Mat. Astr. Fys.* **26A** 1
[3] des Cloizeaux J and Pearson J 1962 *Phys. Rev.* **128** 2131
[4] Griffiths R B 1964 *Phys. Rev.* **133** A768
[5] Ovchinikov A 1969 *Zh. Eksp. Teor. Fiz.* **56** 1354
[6] Takahashi M 1971 *Prog. Theor. Phys.* **46** 401
[7] Faddeev L D and Takhtajan L A 1981 *Zap. Nauchn. Semin. LOMI* **109** 134
[8] Schlottmann P 1985 *Phys. Rev. lett.* **54** 2131; 1986 *Phys. Rev.* B **33** 4880
[9] Takahashi M and Yamada M 1985 *J. Phys. Soc. Japan* **54** 2808
[10] Lee K and Schottmann P 1989 *J. Phys.: Condens. Matter* **1** 2759
[11] Orbach R 1958 *Phys. Rev.* **112** 309
[12] des Cloizeaux J and Gaudin M 1966 *J. Math. Phys.* **7** 1384
[13] Yang C N and Yang C P 1966 *Phys. Rev.* **150** 321, 327
[14] Kulish P P, Reshetekhin N Yu and Sklyanin E K 1981 *Lett. Math. Phys.* **5** 393
[15] Takhtajan L A 1982 *Phys. Lett.* **87A** 479
[16] Haldane F D M 1982 *J. Phys. C: Solid State Phys.* **15** L1309
[17] Avdeev L V and Dörfel B D 1985 *Nucl. Phys.* B **257** 253
[18] Babujian H M 1982 *Phys. Lett.* **90A** 479; 1983 *Nucl. Phys.* B **215** 317
[19] Lee K and Schlottmann P 1987 *Phys. Rev.* B **36** 466
[20] Sutherland B 1975 *Phys. Rev.* B **12** 3795
[21] Andrei N and Johannesson H 1984 *Phys. Lett.* **104A** 370
[22] Johannesson H 1986 *Phys. Lett.* **116A** 113
[23] Schlottmann P 1987 *Phys. Rev.* B **36** 5177
[24] Andrei N and Johannesson H 1984 *Phys. Lett.* **100A** 108
[25] Lee K and Schlottmann P 1988 *Phys. Rev.* B **37** 379
[26] Schlottmann P and Lee K 1990 *Magnetic Properties of Low-Dimensional Systems II* ed L M Falicov, F Mejía-Lira and J L Morán-López (Heidelberg: Springer) p 205
[27] Baxter R J 1972 *Ann. Phys. NY* **70** 193, 323
[28] Yang C N 1967 *Phys. Rev. Lett.* **19** 1312
[29] Andrei N and Destri C 1984 *Phys. Rev. Lett.* **52** 364
[30] Tsvelick A M 1985 *J. Phys. C: Solid State Phys.* **18** 159
[31] Desgranges H U 1985 *J. Phys. C: Solid State Phys.* **18** 5481
[32] Tsvelick A M and Wiegmann P B 1984 *Z. Phys.* B **54** 201
[33] Sacramento P D and Schlottmann P 1991 *Phys. Rev.* B **43** 13294