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The Heisenberg chain with impurities: crossover from Fermi-liquid to non-Fermi-liquid behaviour

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Abstract. We consider an integrable SU(2)-invariant model consisting of a Heisenberg chain of spins S (the Takhtajan–Babujian model) interacting with a finite concentration c of impurity spins S'. The thermodynamic Bethe-*ansatz* equations are stated for this model. The ground-state equations are analysed as a function of c, the magnetic field and the coupling parameter (impurity rapidity p_0) of the impurities to the lattice. In zero field the ground state is a singlet for finite c, but becomes non-Fermi-liquid-like as $c \to 0$ for $S' < S$. Two rapidity bands play a role at $T = 0$ corresponding to strings of length $2S$ and $2S'$, respectively. The van Hove singularities of the empty bands define two critical fields, $H_c(c, p_0)$ and $H_s(c, p_0)$, at which the susceptibility diverges. H_c tends to zero as $c \to 0$ giving rise to a crossover from non-Fermi-liquid behaviour for $H > H_c$ to Fermi-liquid-like behaviour for $H < H_c$. The spectrum of elementary excitations and the finite-size corrections to the ground-state energy are calculated, and used to discuss the asymptotic behaviour of spin–spin correlation functions for long times and large distances.

1. Introduction

There has recently been interest in integrable spin chains containing impurity spins. For the host we consider the Takhtajan–Babujian model [1–3] which is the integrable SU(2)-invariant generalization of the standard Heisenberg chain of spins 1/2 to higher spins S. The model consists of an interaction between spins on nearest-neighbour sites, which has the form of a polynomial in $(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})$ of order $2S$. An isolated impurity of spin S' can either be located on the mth link of the Heisenberg chain [4–6] coupled to both neighbouring sites or at the end of an open chain [7] coupled only to the first or last site of the chain. The interaction between the impurity and the chain is of a special type, constructed such that the model remains integrable (and SU(2) invariant) [4–6].

The model and its solution are constructed from the scattering matrices via the quantum inverse scattering method. The diagonalization of the transfer matrices then yields the Bethe-*ansatz* equations for the spin chain with impurity. For the embedded impurity the condition of integrability leads to a phase shift for forward scattering, but no reflection scattering amplitude. In the case of an impurity in an open-ended chain, on the other hand, the boundary acts as a perfect backscatterer with vanishing transmission. In this case the effects of the boundary and the impurity have to be separated. The magnetic properties of the impurity for small fields do not depend on the location (on a link or at the open end) of the impurity and for large fields the asymptotically free spin is recovered for both cases with the same 'universal' corrections [7].

Three situations have to be distinguished for the integrable spin chain with impurity [6,8,9]:

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(i) If $S' = S$ the impurity is just one more site in the chain. The $T = 0$ entropy vanishes for all fields, giving rise to Fermi-liquid-like behaviour; i.e., the susceptibility is finite and the specific heat is proportional to T.

(ii) If $S' > S$ the impurity spin is only partially compensated at $T = 0$, leaving an effective spin of $S' - S$ that is weakly coupled to the chain. The entropy is singular, i.e., $S(T = 0, H = 0) = \ln[2(S' - S) + 1]$, and $S(T = 0, H \neq 0) = 0$. As a function of T the remaining spin degeneracy gives rise to a Schottky anomaly at about $T \approx H$ and the zero-field susceptibility diverges following a Curie law.

(iii) If $S' < S$ the entropy has an essential singularity at $T = H = 0$, giving rise to critical behaviour, i.e. power laws of H and T, as H and T both tend to zero.

These properties are in close analogy with (i) the completely compensated, (ii) the undercompensated and (iii) the overcompensated impurity spin situations in the multi-channel Kondo problem [9–14].

This singular behaviour appears to be inconsistent with renormalization group studies [15], which conclude that the only stable critical points correspond to an unperturbed (periodic) chain and a chain with a break at the impurity site (the open-ended chain). Only the latter fixed point may have a remnant impurity spin. A more detailed study of the system around the integrable point in parameter space leads to the conclusion that the integrable impurity model corresponds to a non-generic multi-critical point [16].

The situation of an embedded impurity has been extended to a finite concentration c of impurities (a Heisenberg chain of spins 1/2 with impurities of spin S') [17]. This adds one more variable to the parameter space without destroying the integrability of the model. As a function of c it is found that the behaviour for finite c is different from that of the isolated impurity; that is, the system is a two-component Luttinger liquid and the ground state is a singlet. This result is consistent with the conclusion reached from the renormalization group flow diagram [16] that the isolated-impurity model corresponds to a multi-critical fixed point. The mesoscopic corrections to the ground-state energy for the two-component Luttinger liquid and the quantum interference pattern in persistent spin currents as a function of the electric field flux (the Aharonov–Casher effect) have been discussed in reference [18]. This model is also closely related to the chain of alternating spins proposed by de Vega and Woynarovich [19].

In this paper we extend the above results in several ways:

(a) An impurity rapidity p_0 is introduced in analogy to Kondo impurities embedded into Luttinger liquids. The parameter p_0 allows one to continuously vary the coupling strength of the impurities to the host [7, 20–22].

(b) While in reference [17] we considered undercompensated impurities ($S = 1/2, S' > 1/2$), here we focus on overcompensated impurities ($S < S'$). This allows us to study the crossover from Fermi-liquid to non-Fermi-liquid behaviour as a function of c, p_0 and the magnetic field H.

(c) We discuss the spectrum of elementary excitations for the two-component Luttinger liquid (finite c) and the gradual depopulation of the spinon bands as a function of H and the coupling parameter p_0.

(d) We calculate the mesoscopic corrections to the ground-state energy and use them to study the asymptotic behaviour of spin–spin correlation functions for long times and large distances.

The rest of the paper is organized as follows. In section 2 we state the discrete Bethe-*ansatz* equations diagonalizing the model, classify the states and obtain the integral equations determining the thermodynamics and the ground state. The Hamiltonian for an isolated impurity is discussed in the appendix. In section 3 we summarize the results for an isolated

impurity (the generalization of reference [6] to $p_0 \neq 0$). The ground-state properties for $c \neq 0$ are presented in section 4. The evolution of the dressed energy bands for the spinon strings is discussed as a function of H, and the magnetization and the critical fields (corresponding to one-dimensional van Hove singularities) are obtained as a function of c and p_0. The conditions for a crossover from Fermi-liquid to non-Fermi-liquid behaviour are analysed. In section 5 we address the spectrum of elementary excitations. The finite-size corrections to the ground-state energy are calculated in section 6 and then used to obtain the critical exponents of the asymptotics of the spin–spin correlation functions. Conclusions follow in section 7.

2. Bethe-*ansatz* equations

2.1. Vertex weights and the transfer matrix

As in references [1–6], the model is defined by the transfer matrix in terms of the vertex weights. The vertex weight operator $R(\lambda)$ acting on the space of the tensor product of two spins S is defined by

$$_{SS}R^{12}(\lambda) = -\sum_{j=0}^{2S}\prod_{k=1}^{j}\frac{\lambda-k}{\lambda+k}P^j \tag{1}$$

where P^j is a projector that selects the states with total spin j. Hence, if $|l\rangle$ is a state with total spin l, then $P^j|l\rangle = \delta_{j,l}|l\rangle$ and

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

with $x_l = \frac{1}{2}l(l+1) - S(S+1)$ and $x = \boldsymbol{S}_1\cdot\boldsymbol{S}_2$. Hence, $P^j(x)$ is a polynomial of order $2S$ in x. The vertex weights satisfy the triangular Yang–Baxter relation, so the model is integrable. These vertex weights define the Babujian–Takhtajan model of spin S without impurities.

The weight of the vertex between the impurity of spin S' and the host spin S can be constructed by a similar procedure. The result for $S' = 1$ and arbitrary spin S can be found in reference [5]. We limit ourselves to presenting the vertex weight for $S' = \frac{1}{2}$ and arbitrary spin S [1–6]:

$$_{S\sigma}R^{12}(\lambda) = \tfrac{1}{2}\big(1-2\lambda\big)I_1\otimes I_2 + \boldsymbol{S}_1\otimes\boldsymbol{\sigma}_2 \tag{3}$$

where I denotes the identity and the vector Pauli matrices represent the spin S'. This vertex weight satisfies the triangular relation with equation (1), which is sufficient for the integrability of the model.

We now introduce a standard monodromy matrix $\hat{J}(\lambda)$:

$$\hat{J}(\lambda) = {}_{S_0S_1}R^{01}(\lambda)\ {}_{S_0S_2}R^{02}(\lambda)\cdots{}_{S_0S_N}R^{0N}(\lambda) \tag{4}$$

where the matrix product is carried out in the $(2S+1)$-dimensional auxiliary space denoted by S_0. (Note that since we construct an SU(2)-invariant model, the dimension of the auxiliary space is irrelevant. Any value of the spin S_0 yields the same result.) Associated with each vertex weight is a spin, e.g. S_i at the site i, which is either a spin S or an impurity spin S'. There are N_h spins S and N_i spins S', with $N = N_h + N_i$ being the total length of the chain. For an impurity vertex weight we shift the argument λ by the quantity p_0, the impurity rapidity. In principle we may apply a different argument shift to each impurity. We will briefly address the consequences of a distribution of impurity rapidities in section 7.

The trace over the ingoing and outgoing S_0-lines yields the transfer matrix $T(\lambda)$:

$$T(\lambda) = \mathrm{Tr}_0(\hat{J}(\lambda)). \tag{5}$$

The transfer matrices for different values of the spectral parameter λ commute, i.e., there is a basis of states that diagonalizes $T(\lambda)$ for all λ simultaneously. This also holds for any distribution of impurity rapidities p_0. The Hamiltonian, i.e. the energy associated with the transfer matrix, is then constructed according to

$$H = \frac{\mathrm{d}}{\mathrm{d}\lambda} \ln T(\lambda)\bigg|_{\lambda=0}. \tag{6}$$

This procedure leads to the Babujian–Takhtajan Heisenberg chain [1–3] of spins S for $N_i = 0$ (the absence of impurities) and of spin S' for $N_h = 0$ (no host spins). The interaction Hamiltonian for an isolated impurity of arbitrary spin S' with $p_0 = 0$ and $S = 1/2$ was derived in reference [4], for $S = 1$ and $p_0 = 0$ in reference [5] and for the general case ($p_0 = 0$) it is discussed in reference [6]. The construction of the Hamiltonian for $p_0 \neq 0$ is more involved and has been carried out for related models in references [7, 18, 20–22]. A brief discussion is given in the appendix.

The many-impurity Hamiltonian depends on the relative space distribution of the impurity spins and has to be constructed for each particular configuration. For instance, if all impurities are separated from each other by a distance of at least three lattice spaces, the Hamiltonian is just the sum of those of the isolated impurities. In general there are a large number of Hamiltonians (with different space distributions of impurities) corresponding to the same energy eigenvalue. In this integrable model the energy eigenvalues do not depend on the relative positions of the impurities. This peculiar property is the consequence of the integrability or equivalently of the structure of the transfer matrix. Despite this 'locality' structure (lack of dependence on distances and large degeneracy of space configurations), the many-impurity Hamiltonian leads to a singlet ground state, in contrast to the single-impurity Hamiltonian for which the ground state is degenerate. This model is related to the translationally invariant lattice of alternating spins 1/2 and S ($c = 1/2$) with second-next-nearest neighbour interactions considered by de Vega and Woynarovich [19].

2.2. Bethe-ansatz equations

The simultaneous diagonalization of the transfer matrices leads to the Bethe-*ansatz* equations. Following the standard procedure outlined elsewhere [1–6] we obtain

$$\left(\frac{\Lambda_j + \mathrm{i}S}{\Lambda_j - \mathrm{i}S}\right)^{N_h} \left(\frac{\Lambda_j - p_0 + \mathrm{i}S'}{\Lambda_j - p_0 - \mathrm{i}S'}\right)^{N_i} = -\prod_{l=1}^{M} \frac{\Lambda_j - \Lambda_l + \mathrm{i}}{\Lambda_j - \Lambda_l - \mathrm{i}} \tag{7}$$

where $j = 1, \ldots, M$. The Λ_n are the spin rapidities which are related to the wavenumbers of the magnons. The energy and the magnetization are given by

$$\begin{aligned} E &= -J\frac{N_h}{N}\sum_{l=1}^{M}\frac{S}{\Lambda_l^2 + S^2} - J\frac{N_i}{N}\sum_{l=1}^{M}\frac{S'}{(\Lambda_l - p_0)^2 + S'^2} \\ S_z &= \left(N_h S + N_i S'\right) - M. \end{aligned} \tag{8}$$

The concentration of impurities is defined as $c = N_i/N$ and $N_h/N = 1 - c$, where N is the total number of sites. For $c = 0$ or $c = 1$ we recover the Bethe-*ansatz* equations for the Babujian–Takhtajan Heisenberg chains of spins S and S', respectively. Note that the Bethe-*ansatz* equations, the energy and the magnetization are all symmetric under the exchange of (N_i, S', p_0) and $(N_h, S, 0)$, i.e. the interchange of the host and impurities. The energy has

$N_h + N_i$ terms that arise from the N factors of the transfer matrix of which N_h are host scattering matrices and N_i are impurity scattering matrices. This result is independent of the choice of the dimension of the auxiliary spin space S_0. Below we consider the symmetrized version of the above equations, i.e. the case where $c/2$ impurities have a forward rapidity p_0 and $c/2$ have a backward rapidity $-p_0$. This does not require any further consideration, since the model is integrable for any distribution of impurity rapidities.

2.3. Thermodynamics

In the thermodynamic limit the solutions of equation (7) lie in the complex plane and form strings of length $(n-1)$ [3–6, 23]:

$$\Lambda_j^{n,\alpha} = \Lambda_j^n + \mathrm{i}(n+1-2\alpha)/2 \qquad \alpha = 1, \ldots, n \tag{9}$$

where Λ_j^n is a real parameter representing the motion of the centre of mass of the string. The length of the string is in principle arbitrary, $n = 1, 2, \ldots$. If ξ_n is the number of strings of length n, then we must satisfy

$$M = \sum_{n=1}^{\infty} n\xi_n. \tag{10}$$

In general, a string excitation of order n represents a bound-magnon state of n magnons, although exceptions have been found [24] in which string states do not correspond to bound magnons.

The rapidities satisfy Fermi statistics and their occupation is most conveniently described in terms of dressed energies, $\epsilon_n(\Lambda)$, which enter the Fermi distribution function. In thermal equilibrium they satisfy the following integral equations [3–6, 23]:

$$\begin{aligned}\epsilon_m(\Lambda) = T \int \mathrm{d}\Lambda'\, G_0(\Lambda - \Lambda') \ln\left\{\left[1 + \exp(\epsilon_{m-1}(\Lambda')/T)\right]\left[1 + \exp(\epsilon_{m+1}(\Lambda')/T)\right]\right\} \\ - J\pi(1-c)G_0(\Lambda)\delta_{m,2S} - J\pi c\tfrac{1}{2}\left[G_0(\Lambda - p_0) + G_0(\Lambda + p_0)\right]\delta_{m,2S'}\end{aligned} \tag{11}$$

where $G_0(\Lambda) = [2\cosh(\pi\Lambda)]^{-1}$. Equations (11) are the thermodynamic Bethe-*ansatz* equations, which are only complete with the asymptotic field boundary condition

$$\lim_{m\to\infty} \frac{\epsilon_m}{m} = H. \tag{12}$$

The free energy of the system is given by

$$\begin{aligned}F(H,T) = F_0 - NT(1-c)\int \mathrm{d}\Lambda\; G_0(\Lambda)\ln\left[1 + \exp(\epsilon_{2S}(\Lambda)/T)\right] \\ - NTc\int \mathrm{d}\Lambda\; \tfrac{1}{2}\left[G_0(\Lambda - p_0) + G_0(\Lambda + p_0)\right]\ln\left[1 + \exp(\epsilon_{2S'}(\Lambda)/T)\right]\end{aligned} \tag{13}$$

where F_0 is the ground-state energy in zero magnetic field:

$$\begin{aligned}F_0 = \tfrac{1}{2}JN(1-c)^2\left[\psi(\tfrac{1}{2}) - \psi(\tfrac{1}{2}+S)\right] \\ + JNc(1-c)\,\mathrm{Re}\left[\psi(\tfrac{1}{2} + |S-S'| + \mathrm{i}\tfrac{1}{2}p_0) - \psi(\tfrac{1}{2}+S+S'+\mathrm{i}\tfrac{1}{2}p_0)\right] \\ + \tfrac{1}{4}JNc^2\,\mathrm{Re}\left[\psi(\tfrac{1}{2}) + \psi(\tfrac{1}{2}+\mathrm{i}p_0) - \psi(\tfrac{1}{2}+S') - \psi(\tfrac{1}{2}+S'+\mathrm{i}p_0)\right].\end{aligned} \tag{14}$$

ψ is the digamma function and Re denotes the real part.

2.4. Ground-state equations

The ground-state integral equations are obtained in the limit $T \to 0$. From equations (11) we have that as $T \to 0$ only ϵ_{2S} and $\epsilon_{2S'}$ can become negative. Only states with negative dressed energy are populated. After some algebra we arrive at the following coupled integral equations:

$$\begin{aligned}
&\epsilon_{2S}(\Lambda) + \int_{\epsilon_{2S}<0} \mathrm{d}\Lambda'\, K_{2S,2S}(\Lambda-\Lambda')\,\epsilon_{2S}(\Lambda') \\
&\qquad + \int_{\epsilon_{2S'}<0} \mathrm{d}\Lambda'\, K_{2S,2S'}(\Lambda-\Lambda')\epsilon_{2S'}(\Lambda') = 2SH - \pi J g_{2S}(\Lambda) \\
&\epsilon_{2S'}(\Lambda) + \int_{\epsilon_{2S}<0} \mathrm{d}\Lambda'\, K_{2S',2S}(\Lambda-\Lambda')\epsilon_{2S}(\Lambda') \\
&\qquad + \int_{\epsilon_{2S'}<0} \mathrm{d}\Lambda'\, K_{2S',2S'}(\Lambda-\Lambda')\epsilon_{2S'}(\Lambda') = 2S'H - \pi J g_{2S'}(\Lambda)
\end{aligned} \tag{15}$$

where the integration kernels are given by

$$K_{n,n'}(\Lambda) = a_{n+n'}(\Lambda) + 2\sum_{l=1}^{p_{n,n'}} a_{n+n'-2l}(\Lambda) + a_{|n-n'|}(\Lambda) \tag{16}$$

with $a_n(\Lambda) = n/(2\pi)/[\Lambda^2 + (n/2)^2]$, $a_0 \equiv 0$ and $p_{n,n'} = \min(n, n') - 1$. The driving terms are

$$\begin{aligned}
g_{2S}(\Lambda) &= (1-c)\sum_{l=1}^{2S} a_{4S+1-2l}(\Lambda) \\
&\quad + \tfrac{1}{2}c \sum_{l=1}^{2\min(S,S')} \left[a_{2S+2S'+1-2l}(\Lambda - p_0) + a_{2S+2S'+1-2l}(\Lambda + p_0)\right] \\
g_{2S'}(\Lambda) &= (1-c) \sum_{l=1}^{2\min(S,S')} a_{2S+2S'+1-2l}(\Lambda) \\
&\quad + \tfrac{1}{2}c \sum_{l=1}^{2S'} \left[a_{4S'+1-2l}(\Lambda - p_0) + a_{4S'+1-2l}(\Lambda + p_0)\right].
\end{aligned} \tag{17}$$

The density distribution functions for the rapidities, $\rho_{2S}(\Lambda)$ and $\rho_{2S'}(\Lambda)$, and their holes, $\rho_{2S,h}(\Lambda)$ and $\rho_{2S',h}(\Lambda)$, satisfy similar integral equations:

$$\begin{aligned}
&\rho_{2S,h}(\Lambda) + \rho_{2S}(\Lambda) + \int_{\epsilon_{2S}<0} \mathrm{d}\Lambda'\, K_{2S,2S}(\Lambda-\Lambda')\rho_{2S}(\Lambda') \\
&\qquad + \int_{\epsilon_{2S'}<0} \mathrm{d}\Lambda'\, K_{2S,2S'}(\Lambda-\Lambda')\rho_{2S'}(\Lambda') = g_{2S}(\Lambda) \\
&\rho_{2S',h}(\Lambda) + \rho_{2S'}(\Lambda) + \int_{\epsilon_{2S}<0} \mathrm{d}\Lambda'\, K_{2S',2S}(\Lambda-\Lambda')\rho_{2S}(\Lambda') \\
&\qquad + \int_{\epsilon_{2S'}<0} \mathrm{d}\Lambda'\, K_{2S',2S'}(\Lambda-\Lambda')\rho_{2S'}(\Lambda') = g_{2S'}(\Lambda).
\end{aligned} \tag{18}$$

The energy and the magnetization are given by

$$\begin{aligned}
E/N &= -J\pi \int_{\epsilon_{2S}<0} \mathrm{d}\Lambda\; g_{2S}(\Lambda)\rho_{2S}(\Lambda) - J\pi \int_{\epsilon_{2S'}<0} \mathrm{d}\Lambda\; g_{2S'}(\Lambda)\rho_{2S'}(\Lambda) \\
S_z/N &= \left[(1-c)S + cS'\right] - 2S \int_{\epsilon_{2S}<0} \mathrm{d}\Lambda\; \rho_{2S}(\Lambda) - 2S' \int_{\epsilon_{2S'}<0} \mathrm{d}\Lambda\; \rho_{2S'}(\Lambda).
\end{aligned} \tag{19}$$

3. The isolated-impurity limit

In the limit $c \to 0$ only the $n = 2S$ strings are present in the ground state. This means that the system is driven only by the host and not by the impurities. Hence, the integral equations (15) and (18) reduce to single integral equations of the Fredholm type. The properties of isolated impurities for $p_0 = 0$ have been obtained in reference [6]. Below we present the results for an impurity with $p_0 \neq 0$, focusing on the low-T and small-field properties. Again, three situations have to be distinguished: (i) if $S' = S$ the impurity is just one more link in the chain; (ii) if $S' > S$ the impurity is undercompensated; and (iii) if $S' < S$ the impurity is overcompensated.

In zero field the band of $2S$-strings is completely filled and the hole density function $\rho_{2S,h}$ is identically zero. For a small magnetic field the large Λ-tails of the distribution become unpopulated and the Fredholm equations (15) and (18) can be reduced to a hierarchical sequence of Wiener–Hopf integral equations, which can be solved by standard analytical methods. For the small-field magnetization of the impurity, we obtain for the three cases

$$\begin{aligned}
&\text{(i) } S' = S \qquad M_{imp} = (SH/\pi^2 T_K)[1 + S/|\mathcal{L}| - S^2(\ln|\mathcal{L}|)/(\mathcal{L})^2 + \cdots] \\
&\text{(ii) } S' > S \qquad M_{imp} = (S' - S)[1 + S/|\mathcal{L}| - S^2(\ln|\mathcal{L}|)/(\mathcal{L})^2 + \cdots] \\
&\text{(iii) } S' < S \qquad M_{imp} = A(H/T_K)^{1/S}
\end{aligned} \tag{20}$$

where A is a constant that depends on S and S'. Here $T_K = \exp(-\pi|p_0|)$ plays the role of the Kondo temperature (we assumed here a large p_0; otherwise T_K has a different functional dependence) and $\mathcal{L}$ is shorthand notation for $\ln(H/T_K)$. Hence, in case (i) the zero-field susceptibility is finite with logarithmic corrections which are well known for Heisenberg chains [3]. For case (ii) the impurity magnetization is finite, corresponding to an effective spin $S' - S$, which is weakly coupled to the spin waves in the host (the logarithmic corrections signal asymptotic freedom). Finally, for case (iii) the impurity spin is overcompensated, giving rise to critical (non-Fermi-liquid) behaviour. The susceptibility diverges as a power law determined by the host spin. For $S = 1$ and $S' = 1/2$ the divergence is on a logarithmic scale. The difference between the cases where $p_0 = 0$ and $p_0 \neq 0$ is the changed Kondo temperature, i.e. the energy scale, and there is no change in the qualitative behaviour [6].

The properties of the three cases are also reflected in the zero-temperature entropy of the impurity. In a finite field (independent of its magnitude) the entropy vanishes at $T = 0$ in all three cases. This is, however, different for zero field where we have [6]

$$\begin{aligned}
&\text{(i) } S' = S \qquad S_{imp}(T = H = 0) = 0 \\
&\text{(ii) } S' > S \qquad S_{imp}(T = H = 0) = \ln[2(S' - S) + 1] \\
&\text{(iii) } S' < S \qquad S_{imp}(T = H = 0) = \ln\{\sin[\pi(2S' + 1)/(2S + 2)]/\sin[\pi/(2S + 2)]\}.
\end{aligned} \tag{21}$$

Hence, in case (i) the ground state is a singlet (Luttinger liquid) and the entropy is a continuous function of H and T. If $S' > S$ the zero-field entropy is that of the remaining free spin, $S' - S$, which is consistent with the above results for the magnetization. A small magnetic field lifts the degeneracy and the entropy vanishes. For $S' < S$ the zero-field entropy corresponds to a fractional spin and the entropy has an essential singularity at $T = H = 0$ (the quantum critical point). These results are identical to those for the $p_0 = 0$ case [6].

From the Luttinger properties in case (i) it follows that the low-T specific heat is proportional to T. For the undercompensated spin $S' > S$ (case (ii)) the remaining effective free spin, $S' - S$, gives rise to a Schottky anomaly at $T \approx H$. In case (iii) the quantum critical point of the overcompensated spin yields power-law dependences as a function of T:

$$\text{(iii) } S' < S \qquad C_{imp} \propto (T/T_K)^{4/(2S+2)} \qquad T\chi_{imp} \propto (T/T_K)^{4/(2S+2)}. \tag{22}$$

Again the critical exponents depend only on the spin of the host, since it is the host driving the quantum critical point. For $S = 1$ and $S' = 1/2$, instead of critical exponents a logarithmic temperature dependence is obtained:

$$S' = 1/2 \text{ and } S = 1 \qquad C_{imp} \propto (T/T_K)\ln(T_K/T) \qquad T_K\chi_{imp} \propto \ln(T_K/T). \tag{23}$$

Again, the only effect of p_0 is to introduce the Kondo energy scale.

The properties of the impurity in all three cases are closely related to the multi-channel Kondo problem [9–14]. If on the other hand we consider $c \to 1$, only the band of $2S'$-strings is occupied. The properties are then those of a Babujian–Takhtajan chain of spins S' with impurity of spin S and rapidity $-p_0$, i.e. the roles of the impurity and the host are interchanged.

4. Ground-state properties at finite concentration

The properties of the system change dramatically if the concentration of impurities is finite. We consider first the zero-field case, which can be solved analytically, and then we present the numerical results for the system in a finite magnetic field.

4.1. The zero-magnetic-field solution

In zero field the two populated rapidity bands, corresponding to strings of $2S$- and $2S'$-spins, are completely filled. This means that the two dressed energies are negative for all rapidity values Λ. The integral equations (15) and (18) can then be solved by Fourier transformation:

$$\begin{aligned}
\epsilon_{2S}(\Lambda) &= -\frac{\pi J(1-c)}{2\cosh(\pi\Lambda)} \qquad \rho_{2S}(\Lambda) = \frac{(1-c)}{2\cosh(\pi\Lambda)} \\
\epsilon_{2S'}(\Lambda) &= -\frac{\pi Jc}{2}\left\{\frac{1}{2\cosh[\pi(\Lambda-p_0)]} + \frac{1}{2\cosh[\pi(\Lambda+p_0)]}\right\} \\
\rho_{2S'}(\Lambda) &= \frac{c}{2}\left\{\frac{1}{2\cosh[\pi(\Lambda-p_0)]} + \frac{1}{2\cosh[\pi(\Lambda+p_0)]}\right\}.
\end{aligned} \tag{24}$$

All densities for other string lengths are identically zero. For $c \to 0$ the density of $2S'$-strings tends to zero.

Inserting (24) into expression (19) we obtain the zero-field ground-state energy F_0, given by equation (14), and that the magnetization vanishes (the ground state is a singlet) for any combination of S and S'. This contrasts with the results for isolated impurities discussed in the previous section. We have to conclude that the limit $c \to 0$ is singular [17]. Below, we will mainly focus on the overcompensated case, i.e. $S' < S$, which for $c \to 0$ shows non-Fermi-liquid behaviour. We discuss this crossover from Fermi-liquid to non-Fermi-liquid in more detail below.

4.2. Magnetic field dependence

The integral equations (15) and (18) for non-zero magnetic field have to be solved numerically. A field H increases the dressed energies ϵ_{2S} and $\epsilon_{2S'}$, so the large $|\Lambda|$-tails are positive and hence unoccupied. The points at which the dressed energies vanish form the 'Fermi surface' of the model. In zero field the Fermi points lie at $\Lambda = \pm\infty$. The dressed energies gradually increase with H until the bands become unpopulated. For sufficiently small c, first the impurity band is depopulated at the critical field H_c and then at the much larger field H_s the band of $2S$-strings also becomes empty. For fields larger than H_s all spins are aligned and the magnetization is saturated at the value $S_z/N = (1-c)S + cS'$. H_s will be called the saturation field.

As a concrete example we specialize our analysis to $S = 1$ and $S' = 1/2$, which for the isolated impurity yields non-Fermi-liquid behaviour. However, for a finite concentration of impurities the results are similar for other combinations of S and S'. For $p_0 = 0$ the two energy bands have their minima at $\Lambda = 0$. For sufficiently large p_0 the impurity band has two minima located roughly at $\Lambda = \pm p_0$. Increasing p_0 decreases the Kondo temperature and hence the coupling between the two bands. This is seen as follows: for a given field H increasing p_0 makes the impurity band off-resonance with the host rapidities, i.e. the bands are not populated for the same intervals of Λ.

The numerical solution of the integral equations for $c = 0.2$ and $p_0 = 2$ is shown in figure 1 for five fields. Curves (a) correspond to the saturation field H_s, for which both dressed energies are positive for all Λ and $\epsilon_2(0) = 0$. The system has no spinons and the magnetization is saturated. Curves (b) refer to a field intermediate between H_c and H_s. Hence, the impurity band is still empty, but the host band, ϵ_2, is partially filled. Curves (c) represent the dressed energies at the critical field, for which $\epsilon_1(\pm\Lambda_0) = 0$ with $\Lambda_0 \approx p_0$ being the point of the minimum of the ϵ_1-band. Hence, the impurity band is still empty and the host band is partially filled. For curves (d) both bands are partially occupied. Finally, curves (e) correspond to zero field, where both bands are completely filled. Note that the field dependence of the impurity band is much more pronounced than that of the host band. These results are similar to those for impurity bands in strongly correlated electron systems [25, 26].

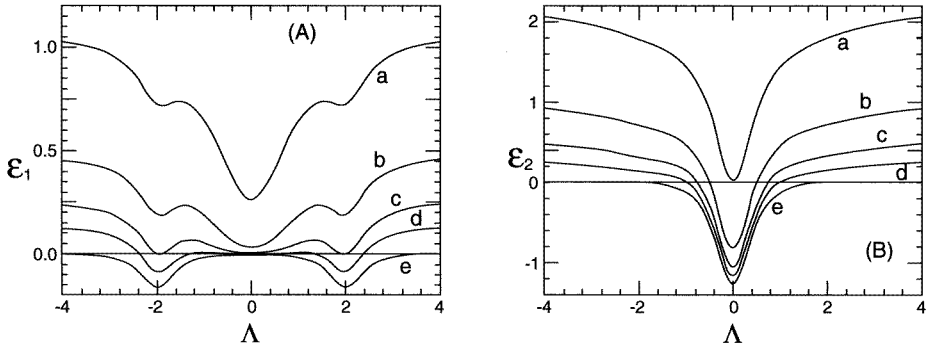

Figure 1. Dressed energy potentials for (A) the impurity band (spinons) and (B) the host band (two-strings of spinons) for a concentration $c = 0.2$ of impurities of spin $S' = 1/2$ and $p_0 = 2$ in a host of spin $S = 1$ for several magnetic fields. The spinons have a three-peak structure arising from the impurity rapidity p_0 (the strength of the coupling of the impurities to the host) and the host two-strings. The curves correspond to (a) $H_s = 1.087$, (b) $H = 0.500$, (c) $H_c = 0.273$, (d) $H = 0.150$ and (e) $H = 0.0$.

The critical and saturation fields as functions of c for three values of p_0 are shown in figure 2(A). The saturation field decreases linearly with the concentration with a slope that increases with p_0. The critical field H_c, on the other hand, increases with c. A larger p_0 decreases the coupling of the impurities to the host (reduces the Kondo temperature), so H_c is reduced with growing p_0. As $c \to 0$ the dependence of H_c on c is non-analytic. This non-analytic behaviour is a consequence of the overscreening of the impurities, and it is absent for $S' > S$ (undercompensated spins; see [17]) where the increase of H_c is linear in c.

For most cases H_c corresponds to the depletion of the impurity band. In figure 2(A) for $p_0 = 0$ the H_c- and H_s-curves intersect at about $c_0 = 0.18$. For $c < c_0$ the critical field refers to the depletion of the ϵ_1-band, while for $c > c_0$ first the ϵ_2-band is depopulated and then the spinon ϵ_1-band at H_s is depopulated.

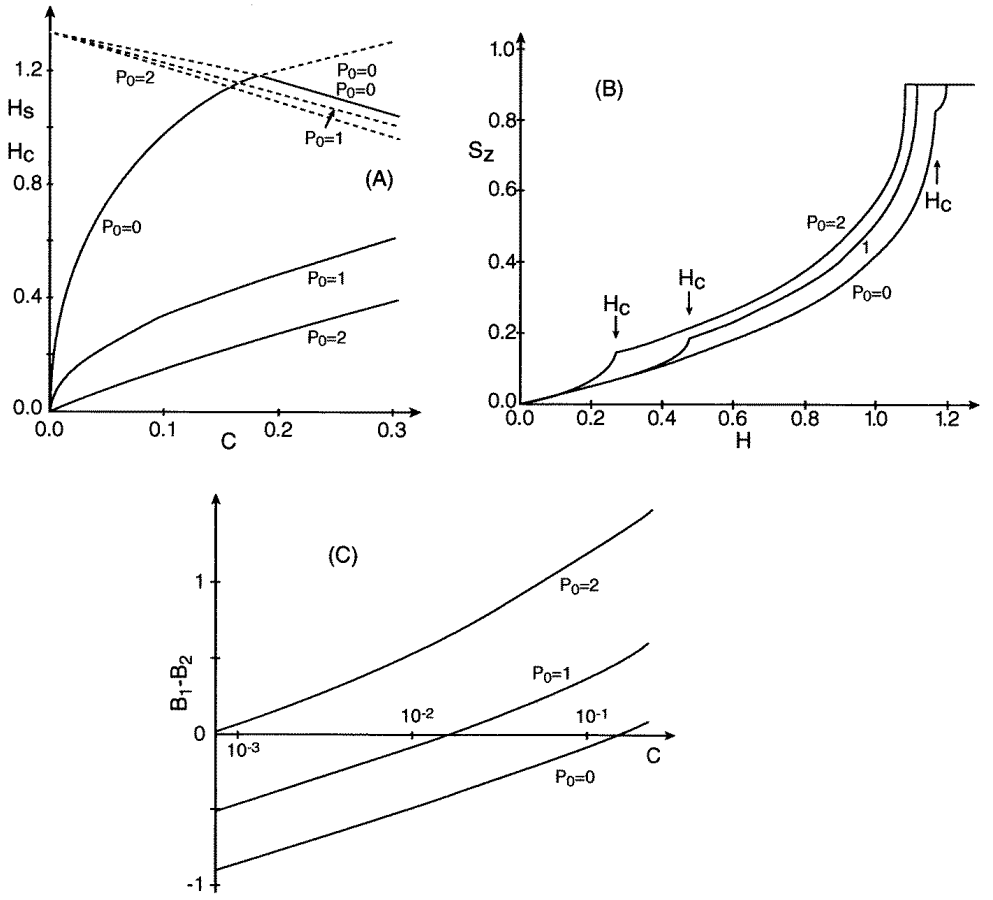

Figure 2. (A) The saturation field H_s (dashed curves) and the critical field H_c (solid curves) as functions of the impurity concentration for $S' = 1/2$ and $S = 1$ and three values of p_0. These are the two fields at which the rapidity bands become empty. H_c depends non-analytically on c as $c \to 0$ as a consequence of the quantum critical point of the isolated-impurity limit. (B) Magnetization as a function of field for $S' = 1/2$, $S = 1$, $c = 0.2$ and for three values of p_0. The susceptibility diverges as the field approaches H_c or H_s from below as a consequence of the one-dimensional van Hove singularity of the empty bands. The magnetization is saturated for fields larger than H_s. For $p_0 = 0$ and as a function of field, first the host band is depleted, while for the other two cases first the impurity band becomes unoccupied. (C) For very small fields the difference of the integration limits $B_1 - B_2$ is independent of the field and depends logarithmically on the concentration.

The magnetization as a function of field is presented in figure 2(B) for $c = 0.2$ and three values of p_0. The magnetization increases monotonically with increasing field and vanishes linearly with the field (the susceptibility is finite for a singlet ground state) as $H \to 0$. The magnetization has cusps at the critical and saturation fields, which arise from the one-dimensional van Hove singularities of the empty bands. The slope of S_z versus H diverges when the critical fields are approached from below. For fields larger then H_s the magnetization is saturated. The curve for $p_0 = 0$ is somewhat different from the other two curves, because in this case the host band is depleted before the impurity band. The low-T specific heat is proportional to the temperature, except at the van Hove singularities, where the leading contribution is $\propto T^{1/2}$.

4.3. The small-magnetic-field limit

For sufficiently small magnetic fields each of the dressed energies, ϵ_{2S} and $\epsilon_{2S'}$, has two zeros, at $\Lambda = \pm B_{2S}$ and $\Lambda = \pm B_{2S'}$, respectively. These are the integration limits for the integral equations (15) and (18). The integration limits are, in principle, functions of the field, the concentration and the impurity rapidity, and tend to infinity as $H \to 0$. The coupled Fredholm equations can be converted into a sequence of coupled Wiener–Hopf equations, from which it is found that, asymptotically for large $|\Lambda|$, the two integral equations for the dressed energies have driving terms that are proportional to each other. This can also be seen from equation (24), where the large $|\Lambda|$-tails of the densities and dressed energies are all exponential and hence proportional to each other. The consequence of this observation is that for small magnetic fields $B_{2S'} - B_{2S}$ is independent of H and only a function of c and p_0. The field is proportional to $\exp(-\pi B_{2S})$, so B_{2S} parametrizes the field.

To obtain $B_{2S'} - B_{2S}$ we numerically solve the integral equations (15). For $S' = 1/2$ and $S = 1$ the result is displayed in figure 2(C) as a function of $\ln(c)$ for three values of p_0. For sufficiently small c the curves are straight lines all with the same slope. The three curves can then be scaled onto each other if we plot $B_1 - B_2$ versus $\ln[c/c_0(p_0)]$, where $c_0(p_0)$ is a scaling constant. We return to this point when we discuss the dressed generalized charges in the context of finite-size corrections to the ground-state energy.

4.4. Crossover from Fermi-liquid to non-Fermi-liquid behaviour

We have learned that for $S' < S$, on the one hand, isolated impurities have a quantum critical point with non-Fermi-liquid properties, while on the other hand, if $c \neq 0$ the ground state is a singlet. The difference between the two situations is the population of the $2S'$-string band, which transforms a one-component Luttinger liquid into one with two components (two kinds of strings). In this subsection we consider the gradual crossover between the two situations as a function of a magnetic field.

Consider first equation (18) for $H > H_c$ for sufficiently small c. In this case the impurity band is empty, so we have one integral equation of the Fredholm type. The driving term can be divided into one for the host (proportional to $(1 - c)$) and one for the impurities (proportional to c). Neglecting the $(1 - c)$-factor the host density is then identical to the pure SU(2)-invariant Heisenberg host chain. The integral equation for the impurity part is identical to the one considered in section 3, except for the constant factor $c = N_i/N$. Hence, for $H_c \ll H \ll T_K$ the impurities have the same non-Fermi-liquid properties as isolated impurities, i.e. a susceptibility that increases as the field is lowered.

At $H = H_c$ the susceptibility is singular, because of the van Hove singularity of the empty $\epsilon_{2S'}$-band. This band is partially filled for $H < H_c$ and yields a two-component Luttinger liquid. Hence, when the divergence of the susceptibility as H_c is approached from below, χ decreases with decreasing field and reaches a finite value as $H \to 0$ (the singlet ground state). In other words, as a function of field the system undergoes a crossover from non-Fermi-liquid properties for $H > H_c$ to Fermi-liquid-like behaviour for $H < H_c$.

5. The excitation spectrum

In this section we derive the spectrum of elementary excitations from the zero-field ground state. For finite c and $H = 0$ both bands are completely filled without hole states. A hole state is obtained by removing one rapidity. To remove the rapidity Λ_0, e.g. corresponding to a $2S$-string of spin waves, requires the excitation energy $\Delta E_{2S}(\Lambda_0)$ and a physical momentum

$p_{2S}(\Lambda_0)$ given by

$$\Delta E_{2S}(\Lambda_0) = |\epsilon_{2S}(\Lambda_0)| \qquad p_{2S}(\Lambda_0) = 2\pi \int_{-\infty}^{\Lambda_0} \mathrm{d}\Lambda \, \left[\rho_{2S}(\Lambda) + \rho_{2S,h}(\Lambda)\right] \tag{25}$$

and similarly for excitations within the $2S'$-band. The excitations are all of the hole type, since the bands are filled.

Using the solutions for the dressed energies and densities derived in section 4.1, we obtain

$$\begin{aligned}
\Delta E_{2S}(\Lambda_0) &= \frac{\pi J(1-c)}{2\cosh(\pi\Lambda_0)} \\
p_{2S}(\Lambda_0) &= 2(1-c)\arctan\left[\exp(\pi\Lambda_0)\right] \\
\Delta E_{2S'}(\Lambda_0) &= \frac{\pi Jc}{4\cosh[\pi(\Lambda_0 - p_0)]} + \frac{\pi Jc}{4\cosh[\pi(\Lambda_0 + p_0)]} \\
p_{2S'}(\Lambda_0) &= c\arctan\{\exp[\pi(\Lambda_0 - p_0)]\} + c\arctan\{\exp[\pi(\Lambda_0 + p_0)]\}\,.
\end{aligned} \tag{26}$$

The range for the physical momentum of the excitations is limited to the intervals $0 \leqslant p_{2S} \leqslant \pi(1-c)$ and $0 \leqslant p_{2S'} \leqslant \pi c$, respectively. Note that in zero field the excitations from the host band do not depend on the impurity rapidity p_0.

The excitation spectrum is shown in figure 3 for $c = 0.2$, $S' = 1/2$, $S = 1$ and several values of p_0. While the excitations from the host band are identical to those of the Babujian–Takhtajan Heisenberg chain rescaled by the factor $1 - c$, the excitations from the impurity band strongly depend on c (<0.5) and the coupling between the host and the impurities, i.e. on p_0. For $p_0 = 0$ the hole excitations from the impurity band again scale with those of the Heisenberg chain if the energy and momentum are multiplied by c. For the Heisenberg chain without impurities the momentum range in zero field is π. This is still the case for the chain with impurities if the ranges of the two excitations are added together. With increasing p_0 the excitations from the impurity band gradually acquire a two-peak structure, which for large p_0 (when T_K is small and the two bands are off-resonance) reduces to a halving of the period.

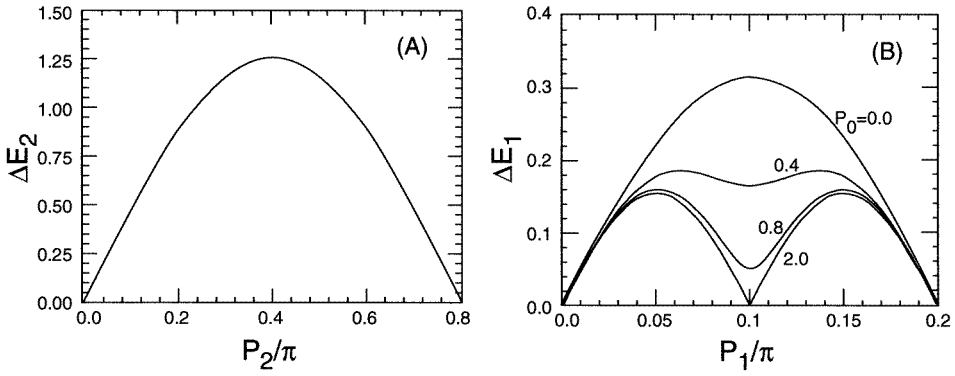

Figure 3. The energy dispersion for the hole excitations from (A) the host band of $2S$-strings and (B) the impurity band of $2S'$-strings for $S' = 1/2$, $S = 1$, $c = 0.2$ and various values of p_0. Note that the excitations of the host depend neither on p_0 nor on S. The two bands decouple with increasing p_0 and for sufficiently large p_0 the period of the impurity band is halved.

Since the spectrum of elementary excitations of the Babujian–Takhtajan Heisenberg chain does not depend on the spin, the excitations shown in figure 3 are independent of S and S'. For small momentum transfer the excitation energy is proportional to the momentum, the proportionality constant being the spin-wave velocity v. The spin-wave velocity in zero field is independent of the spin, so $v = \pi J/2$ for both bands.

6. Finite-size corrections and correlation functions

In this section we first derive the finite-size corrections to the ground-state energy and then we use the low-energy excitation spectrum to study the asymptotics of the spin–spin correlation functions.

6.1. Finite-size effects

The finite size of a ring manifests itself in several ways:

(i) Impurities are important in mesoscopic systems, since their contribution to extensive quantities can become large and observable, and may even change the properties.

(ii) The finite length of a ring yields persistent currents with oscillation periods given by interference patterns of the Aharonov–Casher type.

(iii) Finite-size corrections to the energy determine the critical exponents of the asymptotic dependence at long times and large distances of correlation functions via conformal field theory [27–30].

To calculate the finite-size corrections to the ground-state energy, i.e. the change of the energy due to the finite length of the ring, we follow the procedure developed in references [27] and [31]. We confine ourselves to considering the situation without an applied magnetic field. The ground-state energy including mesoscopic terms is given by

$$E = N\epsilon_\infty + \sum_l \frac{2\pi v^{(l)}}{N}\left[\frac{1}{2}\sum_q (\hat{z}^{-1})_{lq}\,\Delta M^{(q)}\right]^2 + \sum_l \frac{2\pi v^{(l)}}{N}\left\{\left[\sum_q z_{lq}\left(D^{(q)} + \vartheta^{(q)}\right)\right]^2 - \frac{1}{12} + n^{(l)+} + n^{(l)-}\right\} \tag{27}$$

where ϵ_∞ is the ground-state energy density in the thermodynamic limit, l and q label the two bands and can take the values $2S'$ and $2S$, and the $v^{(l)}$ denote the spin-wave velocities for the two bands (in zero field they are both equal to $\pi J/2$). The quantities $\vartheta^{(q)}$ are phase shifts of the Aharonov–Casher type, which could be induced by a radial electric field flux. These phase shifts are not relevant in the present context (for a discussion see reference [18]) and will be neglected.

The mesoscopic energy depends on several quantum numbers. $\Delta M^{(q)}$ is the departure of the number of strings in the band q from the equilibrium value. $D^{(q)}$ is the backward scattering quantum number, i.e. $2D^{(q)}$ represents the difference of forward- and backward-moving strings from the equilibrium value. These quantities are sensitive to the parity in each set of rapidities. Finally, the $n^{(q)\pm}$ define the low-lying excitations about each of the Fermi points. Here $\Delta M^{(q)}$, $n^{(q)\pm}$ and $2D^{(q)}$ always take integer values; hence $D^{(q)}$ can be either an integer or a half-integer depending on the initial conditions.

The quantities z_{lq} in equation (27) are the dressed generalized charges of the excitations at the Fermi points, $z_{lq} = \xi_{l,q}(B_q)$. The dressed charges are determined by the following set of integral equations:

$$\xi_{l,q}(\Lambda) = \delta_{l,q} - \int_{-B_{2S}}^{B_{2S}} \mathrm{d}\Lambda'\; K_{q,2S}(\Lambda - \Lambda')\,\xi_{l,2S}(\Lambda') - \int_{-B_{2S'}}^{B_{2S'}} \mathrm{d}\Lambda'\; K_{q,2S'}(\Lambda - \Lambda')\,\xi_{l,2S'}(\Lambda') \tag{28}$$

where the B_q are the Fermi points determined by the zeros of ϵ_{2S} and $\epsilon_{2S'}$ in the limit $H \to 0$ (see subsection 4.3). In equation (27), $\hat{z}^{-1}$ denotes the inverse of the matrix of dressed generalized

charges. The dressed charges describe the interplay of the different Fermi points when rapidities are added or removed.

The driving terms of equation (28) do not depend on c and p_0. Hence, the only dependence on the physical parameters of the model enters through $B_{2S'} - B_{2S}$, which is field independent but a function of c and p_0. B_{2S} parametrizes the magnetic field and tends to infinity as $H \to 0$. Hence, we may use a plot like figure 2(C) to obtain $B_{2S'} - B_{2S}$ for a given c and p_0. The scaling of the curves for different p_0-values in the limit $H \to 0$ indicates that the dressed charges as functions of c are all similar for the different p_0-parameters.

We solved equation (28) numerically for $S' = 1/2$ and $S = 1$ as a function of $B_1 - B_2$ in the limit of large B_2, since here we only consider the zero-field case. The four dressed generalized charges are shown in figure 4(A). From the form of the integral equations it is clear that z_{11} and z_{22} are always positive, while z_{12} and z_{21} are negative. As $B_1 - B_2 \to -\infty$ the spectral weight of the impurity band tends to zero; in this limit $z_{11} \to 1$, $z_{12} \to 0$, $z_{21} \to -0.5$ and $z_{22} \to 0.5$. For $B_1 - B_2 \to +\infty$, on the other hand, the spectral weight of the host band tends to zero, and in this limit $z_{11} = -z_{12} = 1/\sqrt{2}$, $z_{21} \to 0$ and $z_{22} \to 0.722$. All of the limiting values except the latter can be obtained analytically. z_{22} for $B_1 - B_2 \to +\infty$ has to be determined numerically since the two integral equations do not decouple in that limit.

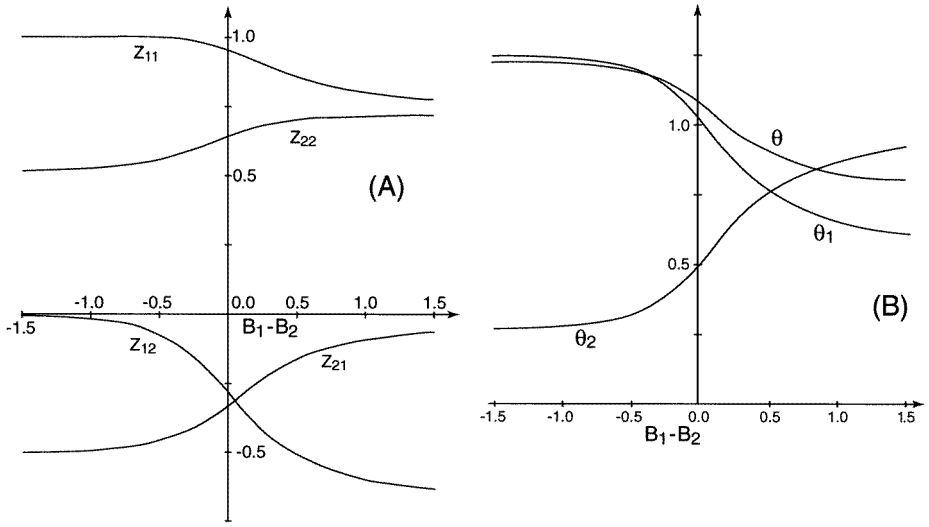

Figure 4. (A) Dressed generalized charges and (B) critical exponents of the spin–spin correlation functions for $S' = 1/2$ and $S = 1$ as functions of $B_1 - B_2$.

In terms of the quantum numbers defined above, the momentum of the system is given by

$$P = \frac{2\pi}{N} \sum_{l=1,2} \left[M^{(l)} \left(D^{(l)} + \vartheta^{(l)} \right) + n^{(l)+} - n^{(l)-} \right]. \tag{29}$$

Equations (27) and (29) define the mesoscopic corrections to the ground-state energy and momentum of a two-component Luttinger liquid.

6.2. Correlation functions

We now obtain the long-time large-distance asymptotics for the longitudinal and transverse spin–spin correlation functions for both the impurity and host bands. As usual for gapless

one-dimensional systems (Luttinger liquids), the correlations fall off as power laws in time and distance. The critical exponents follow from conformal field theory in combination with the finite-size excitation spectrum. In terms of the conformal dimensions of a primary field $\varphi(Q)$, the excitation energy and momentum are given by

$$\begin{aligned} E_{exc}(Q) - E_0 &= \frac{2\pi v^{(2S')}}{N}(\Delta^+_{2S'} + \Delta^-_{2S'}) + \frac{2\pi v^{(2S)}}{N}(\Delta^+_{2S} + \Delta^-_{2S}) \\ P_{exc}(Q) - P_0 &= \frac{2\pi}{N}(\Delta^+_{2S'} - \Delta^-_{2S'} + \Delta^+_{2S} - \Delta^-_{2S}). \end{aligned} \tag{30}$$

Comparing these expressions with equations (27) and (29), we have that

$$\begin{aligned} 2\Delta^\pm_{2S'} = \Bigg\{ &\frac{1}{2\det}\left[z_{2S,2S}\Delta M^{(2S')} - z_{2S,2S'}\Delta M^{(2S)}\right] \\ &\pm \left[z_{2S',2S}D^{(2S)} + z_{2S',2S'}D^{(2S')}\right]\Bigg\}^2 + 2n^{(2S')\pm} \\ 2\Delta^\pm_{2S} = \Bigg\{ &\frac{1}{2\det}\left[z_{2S',2S'}\Delta M^{(2S)} - z_{2S',2S}\Delta M^{(2S')}\right] \\ &\pm \left[z_{2S,2S}D^{(2S)} + z_{2S,2S'}D^{(2S')}\right]\Bigg\}^2 + 2n^{(2S)\pm} \end{aligned} \tag{31}$$

where 'det' is the determinant of the matrix $\hat{z}$. From an inspection of the discrete Bethe-*ansatz* equations it follows that $2D^{(2S')} = \Delta M^{(2S')}$ (mod 1) and $2D^{(2S)} = \Delta M^{(2S)}$ (mod 1), in complete analogy to the case of the usual Heisenberg chain.

The asymptotic form of the correlation function for the operator $\varphi(x,t)$ is [28–30]

$$\begin{aligned} \langle\varphi(x,t)\varphi(0,0)\rangle = &\sum_Q B(Q)\exp\left[-2\mathrm{i}x\left(p_{2S'}D^{(2S')} + p_{2S}D^{(2S)}\right)\right] \\ &\times (x - \mathrm{i}v^{(2S')}t)^{-2\Delta^+_{2S'}}(x + \mathrm{i}v^{(2S')}t)^{-2\Delta^-_{2S'}}(x - \mathrm{i}v^{(2S)}t)^{-2\Delta^+_{2S}}(x + \mathrm{i}v^{(2S)}t)^{-2\Delta^-_{2S}} \end{aligned} \tag{32}$$

where the index Q refers to the conformal fields contained in the operator φ, and $p_{2S'}$ and p_{2S} are the Fermi momenta of the two bands. In zero field the two group velocities are equal, so the four x- and t-dependent factors can be combined into two, and $2p_{2S'} = \pi c$ and $2p_{2S} = \pi(1-c)$.

Consider first the longitudinal spin–spin correlation functions. Since the operators S'_z and S_z do not flip spins, $\Delta M^{(2S')} = \Delta M^{(2S)} = 0$ and $D^{(2S')}$ and $D^{(2S)}$ are integers. The leading term corresponds to $D^{(2S')} = D^{(2S)} = 0$ and one of the four quantum numbers $n^{(2S')\pm}$ and $n^{(2S)\pm}$ being equal to one. The next-to-leading terms involve either $D^{(2S')}$ or $D^{(2S)}$ being equal to one and all other quantum numbers equal to zero. The third-order terms either double the period of oscillation or produce an interference between the Fermi surfaces of the two bands. Period doubling involves either $D^{(2S')}$ or $D^{(2S)}$ being equal to two and all other quantum numbers equal to zero. Interference terms arise from $D^{(2S')} = D^{(2S)} = 1$ (the sum of periods) or $D^{(2S')} = -D^{(2S)} = 1$ (the difference of periods) and all other quantum numbers equal to zero. The leading-order, next-to-leading-order and third-order terms yield for the operator S_z

$$\begin{aligned} \langle S_z(x,t)S_z(0,0)\rangle = &A_S\frac{x^2 - v^2t^2}{(x^2+v^2t^2)^2} + B_S\frac{\cos[\pi(1-c)x]}{(x^2+v^2t^2)^{\theta_S}} + B_{S'}\frac{\cos(\pi cx)}{(x^2+v^2t^2)^{\theta_{S'}}} \\ &+ C_S\frac{\cos[2\pi(1-c)x]}{(x^2+v^2t^2)^{4\theta_S}} + C_{S'}\frac{\cos(2\pi cx)}{(x^2+v^2t^2)^{4\theta_{S'}}} \\ &+ C_+\frac{\cos(\pi x)}{(x^2+v^2t^2)^{\theta_+}} + C_-\frac{\cos[\pi(1-2c)x]}{(x^2+v^2t^2)^{\theta_-}}. \end{aligned} \tag{33}$$

The exponents θ_S and $\theta_{S'}$ are given by

$$\theta_S = z^2_{2S,2S} + z^2_{2S',2S} \qquad \theta_{2S'} = z^2_{2S,2S'} + z^2_{2S',2S'} \tag{34}$$

and are displayed in figure 4(B) for $S' = 1/2$ and $S = 1$ as functions of $B_1 - B_2$. The exponents of the interference terms are

$$\theta_\pm = (z_{2S,2S} \pm z_{2S,2S'})^2 + (z_{2S',2S} \pm z_{2S',2S'})^2. \tag{35}$$

An expression analogous to equation (33) holds for the operator S'_z. The terms included in equation (33) are allowed by symmetry, but their coefficients could be zero. For instance, it is not meaningful to have non-zero $A_{S'}$, $B_{S'}$ and $C_{S'}$ in the S_z-correlation function. Similarly, A_S, B_S and C_S should be zero for the S'_z-correlation function.

We consider now the transverse correlation functions. The operator S_x changes the number of rapidities in the host band by one unit, i.e. $\Delta M^{(2S)} = \pm 1$ and $D^{(2S)} = \pm 1/2$, while all other quantum numbers are zero for the leading term of the correlation function:

$$\langle S_x(x,t) S_x(0,0)\rangle = A\,\frac{2x\cos[\pi(1-c)x/2]}{(x^2+v^2t^2)^{\theta+1/2}}. \tag{36}$$

Similarly, S'_x changes the number of rapidities in the impurity band by one unit, i.e. $\Delta M^{(2S')} = \pm 1$ and $D^{(2S')} = \pm 1/2$, while all other quantum numbers are zero for the leading term:

$$\langle S'_x(x,t) S'_x(0,0)\rangle = A\frac{2x\cos[\pi cx/2]}{(x^2+v^2t^2)^{\theta+1/2}}. \tag{37}$$

The transverse correlation functions of the two bands only differ by the periodicity of their Fermi surface. Here θ is given by

$$\theta = \frac{1}{4\det^2}\theta_{S'} + \frac{1}{4}\theta_S \tag{38}$$

and is shown in figure 4(B) for $S' = 1/2$ and $S = 1$ as a function of $B_1 - B_2$.

7. Concluding remarks

We considered the SU(2)-invariant generalization of the Heisenberg chain of spins S (the Babujian–Takhtajan model) with a finite concentration c of impurities of spin S'. The model is integrable by construction as a function of four parameters, namely S, S', c and the impurity rapidity p_0, which determines the coupling of the impurities to the lattice. We stated the Bethe-*ansatz* equations diagonalizing the model and derived the thermodynamic and ground-state integral equations.

In the isolated-impurity limit we have to distinguish three different situations:

(i) If $S' = S$ the impurity adds just another link to the chain and its low-T properties are those of a Luttinger liquid, i.e. the susceptibility is finite and the specific heat is proportional to T.

(ii) If $S' > S$ the impurity is undercompensated by the lattice spins, leaving a remnant spin of $S' - S$.

(iii) For $S' < S$ the impurity spin is overcompensated giving rise to a quantum critical point and power-law dependences as functions of field and temperature in the susceptibility and the specific heat.

The coupling parameter p_0 introduces an energy scale analogous to the Kondo temperature. The three cases discussed above are in complete analogy with the multi-channel Kondo problem. It has been argued [16] that the this integrable isolated-impurity model corresponds to a non-generic multi-critical fixed point.

A finite concentration of impurities dramatically changes the physical low-T properties of the model for $S' \neq S$. The ground state is a singlet in all cases and the low-T fixed point is given by a two-component Luttinger liquid. As a function of the magnetic field, the two rapidity bands are gradually depleted. For small c first the impurity band is emptied at a critical field H_c and then the host rapidity band is emptied at the saturation field H_s. For $H \geqslant H_s$ all of the spins are aligned and the ground state is ferromagnetic.

For $S' \neq S$ and $H_c < H < T_K$, i.e. for small impurity concentrations, only the host rapidity band is populated (strings of length $2S$) and the properties of the impurities are the same as those of isolated impurities multiplied by the concentration. If $S' < S$ the system then approaches the quantum critical point as the field is reduced (power-law behaviour, unless $S' = 1/2$ and $S = 1$, where the dependence is logarithmic) until H_c is reached. In this regime the impurities are exclusively driven by the host band. At H_c the impurity band becomes partially occupied and this drastically changes the properties. The system is now a two-component Luttinger liquid. At H_c the one-dimensional van Hove singularity of the impurity band gives rise to a square-root divergence in the susceptibility as H_c is approached from below. As the field is lowered further the susceptibility approaches a constant. Hence, as the field is reduced through H_c the system undergoes a crossover from non-Fermi behaviour to Fermi-liquid-like behaviour.

We studied the zero-field spectrum of elementary excitations for the two-band system. Each of the excitations is of the hole type and corresponds to removing one rapidity from one of the bands. The energy and momentum of the excitations of the host band are independent of p_0 and are just those of the standard Heisenberg chain multiplied by $1 - c$. The spectrum of the impurity band strongly depends on the coupling parameter p_0. For small p_0 it scales (the scaling factor is the concentration) with the excitations of the ordinary Heisenberg chain. For large p_0, on the other hand, the period of the spectrum is halved. In zero field the two bands have the same group velocity for the spin waves. This changes if the field is non-zero.

The finite-size corrections to the ground-state energy were obtained in section 6. In zero field they correspond to a two-component Luttinger liquid with the Fermi points at $|\Lambda| \to \infty$. The low-energy excitations are described in terms of quantum numbers representing the changes in the populations of the bands, the backward-scattering quantum numbers and excitations about the four Fermi points. These excitations and the expression for the momentum in terms of the quantum numbers yield the conformal dimensions of the primary fields and hence the critical exponents for the asymptotics of the correlation functions. We studied the longitudinal and transverse spin–spin correlation functions for each band. The critical exponents depend on c and p_0 through the difference of the integration limits $B_{2S'} - B_{2S}$. Terms oscillating as a function of the distance are obtained. The periodicities depend on the Fermi momenta of the two bands, i.e. on the impurity concentration. Third-order terms in the longitudinal correlation function give rise to period doubling and interference of the two Fermi surfaces.

In summary, we studied this interesting model in detail, since it is exactly soluble and it shows explicitly the crossover from non-Fermi-liquid to Fermi-liquid behaviour as a function of c and p_0, which are two model parameters that can be varied continuously. In section 2 we mentioned that the model is integrable for an arbitrary distribution of impurity rapidities. A distribution of p_0 induces a distribution of Kondo temperatures, which may also give rise to non-Fermi-liquid behaviour [32]. Distributions of Kondo temperatures in the context of integrable systems have been discussed in references [25, 33]. For the present model non-Fermi-liquid behaviour can be obtained even in the two-component Luttinger-liquid regime if the distribution of p_0 has a tail tending to infinity. Large values of p_0 yield small values of T_K, i.e. small Fermi energies, and hence eventually a quantum critical point at $T = H = 0$.

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Appendix. The impurity Hamiltonian

The lattice Hamiltonian can be obtained as the logarithmic derivative of the transfer matrix (5); see equation (6). For the single-impurity model the transfer matrix consists of $N-1$ host scattering matrices and one scattering matrix for the host spins and the impurity. The former gives rise to the Hamiltonian of the Babujian–Takhtajan Heisenberg chain [3], where we denote as $H_{i,i+1}$ the interaction for the link between the sites i and $i+1$:

$$H = \sum_{i=1}^{N-1} H_{i,i+1}.$$

We now assume that the impurity is at the site N. By construction, the impurity then interacts with the neighbouring sites $i = 1$ and $i = N-1$. The general structure of the impurity Hamiltonian is now of the following form:

$$\begin{aligned} H_{imp} = {} & f_1(S', p_0)\Big(H^{(S')}_{N-1,N} + H^{(S')}_{N,1} + \{H^{(S')}_{N-1,N}, H^{(S')}_{N,1}\}\Big) \\ & + f_2(S', p_0)H_{N-1,1} + \mathrm{i} f_3(S', p_0)\Big[(H^{(S')}_{N-1,N} + H^{(S')}_{N,1}), H_{N-1,1}\Big] \end{aligned} \tag{A.1}$$

where $f_1(S', p_0)$ and $f_2(S', p_0)$ are even functions of p_0, while $f_3(S', p_0)$ is an odd function of p_0. Here the square (curly) brackets denote a commutator (anticommutator). The Hamiltonian $H^{(S')}_{N,1}$ (and similarly $H^{(S')}_{N-1,N}$) is a polynomial of order $\min(2S, 2S')$ of $(\boldsymbol{S}'_N \cdot \boldsymbol{S}_1)$; e.g. for $S' = 1/2$ (parametrized by Pauli matrices) we have

$$H^{(S'=1/2)}_{N,1} = a(p_0) + b(p_0)(\boldsymbol{\sigma}_N \cdot \boldsymbol{S}_1). \tag{A.2}$$

The interaction Hamiltonian (A.1) involves the spins of the three sites involved. Due to the impurity rapidity p_0 being non-zero, the impurity Hamiltonian breaks the time-reversal (T) and parity (P) symmetries separately, but their product TP is conserved. This manifests itself in a non-zero total quasi-momentum of the system. Note that, by construction, from the integrability condition the impurity involves only forward scattering (unitary transmission) and that the reflected wave has zero amplitude. This makes the model non-generic. It is well known that non-Fermi-liquid properties can only arise in special non-generic situations, while normally a one-dimensional system is a Luttinger liquid.

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