

Integrable spin-1 Heisenberg chain with impurity

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We construct an integrable SU(2)-invariant model consisting of the Heisenberg chain of spin 1 interacting with an impurity of spin S . This generalizes previous results by Andrei and Johannesson for the spin- $\frac{1}{2}$ chain. The model Hamiltonian is diagonalized and the thermodynamics is obtained. For ferromagnetic coupling at low temperatures the impurity susceptibility diverges as T^{-2} and the impurity specific heat is proportional to $T^{1/2}$ for all values of the impurity spin S . For antiferromagnetic coupling and $T=0$ the impurity susceptibility diverges proportionally to $|\ln H|$ as $H \rightarrow 0$ if $S = \frac{1}{2}$, while if $S > 1$ the impurity spin is only partially compensated for by the $S = 1$ chain.

Since Bethe proposed a procedure¹ (now known as Bethe ansatz) to diagonalize the Hamiltonian for the isotropic spin- $\frac{1}{2}$ Heisenberg chain, many important properties for this model have been obtained in numerous contributions.²⁻⁹ Several integrable generalizations of the isotropic $S = \frac{1}{2}$ Heisenberg chain were found: (a) the anisotropic chain,¹⁰⁻¹² (b) the SU(2)-invariant chain of arbitrary spin S ,¹³⁻¹⁷ (c) systems of arbitrary number of components and SU(N) symmetry,¹⁸⁻²⁰ and (d) the spin- $\frac{1}{2}$ Heisenberg chain with an impurity²¹ of arbitrary spin S . In this paper we construct the Hamiltonian of the spin-1 chain with SU(2) symmetry interacting with an impurity of arbitrary spin S , extending in this way the work by Andrei and Johannesson.²¹

The spin-1 chain with SU(2) invariance in the absence of impurity is given by

$$\mathcal{H}_0 = \sum_{n=1}^N \mathcal{H}_{n,n+1} = \frac{J}{4} \sum_{n=1}^N [(\mathbf{S}_n \cdot \mathbf{S}_{n+1}) - (\mathbf{S}_n \cdot \mathbf{S}_{n+1})^2], \quad (1)$$

where S_n are spin-1 operators, N is the length of the chain, and periodic boundary conditions are assumed, $S_{N+1} = S_1$. The impurity is assumed to be located on the m th link, i.e., between the m th and $(m+1)$ th sites, and interacts with both neighboring sites. The interaction must be of a special type to preserve the integrability of the model. If the impurity spin S equals 1, the system reduces to a homogeneous chain of $(N+1)$ links. The form of the interaction is given below.

Following, for instance, Refs. 13, 14, 17, and 21 we consider a set of commuting transfer matrices $T(\lambda)$ yielding the Hamiltonian according to the relation

$$\mathcal{H} = - \frac{J}{2} T(0)^{-1} \frac{dT(\lambda)}{d\lambda} \Big|_{\lambda=0} = \mathcal{H}_0 + \mathcal{H}_{\text{int}}. \quad (2)$$

Note that \mathcal{H} and $T(\lambda)$ commute for all values of λ . The transfer matrix $T(\lambda)$ is obtained as the trace over a matrix product carried out in the auxiliary space V_0 (space of spin 1)

$$T(\lambda) = \text{Tr}_0 [R_{0,N}^{(1)}(\lambda) R_{0,N-1}^{(1)}(\lambda) \cdots R_{0,m+1}^{(1)}(\lambda) R_{0,(m,S)}^{(S)}(\lambda) R_{0,m}^{(1)}(\lambda) \cdots R_{0,1}^{(1)}(\lambda)]. \quad (3)$$

The matrices $R_{0,j}^{(1)}$ are local vertex weights acting on the space built up by the direct product of the auxiliary space V_0 and the local space V_j carrying the spin S_j of the j th site. A necessary and sufficient condition for the commutativity of the transfer matrices for different λ values is the Yang-Baxter triangular relation^{22,23}

$$R_{1,2}(\lambda) R_{1,3}(\lambda + \mu) R_{2,3}(\mu) = R_{2,3}(\mu) R_{1,3}(\lambda + \mu) R_{1,2}(\lambda). \quad (4)$$

A quite general solution for these matrices valid for arbitrary spin spaces has been given in Ref. 13. Specializing their result for SU(2) and all spins equal to 1, we obtain for $R_{0,j}^{(1)}(\lambda)$

$$R_{0,j}^{(1)}(\lambda) = (2 + \lambda - \lambda^2) + 2(\lambda - 1) \mathbf{S}_0 \cdot \mathbf{S}_j - 2(\mathbf{S}_0 \cdot \mathbf{S}_j)^2. \quad (5)$$

This vertex weight generates the Hamiltonian (1) in the absence of impurity.

A second vertex weight, $R_{0,(m,S)}^{(S)}$, is needed to introduce the impurity. In order to preserve the integrability the vertex $R_{0,S}^{(S)}(\lambda)$ (note that the index m only indicates its location in the lattice) is required to satisfy the triangular relation

$$R_{1,2}^{(S)}(\lambda) R_{1,3}^{(1)}(\lambda + \mu) R_{2,3}^{(S)}(\mu) = R_{2,3}^{(S)}(\mu) R_{1,3}^{(1)}(\lambda + \mu) R_{1,2}^{(S)}(\lambda). \quad (6)$$

It is easy to verify that

$$R_{S_0, S}^{(s)}(\lambda) = [S(S+1) + \lambda - \lambda^2] + 2(\lambda - 1)\mathbf{S}_0 \cdot \mathbf{S} - 2(\mathbf{S}_0 \cdot \mathbf{S})^2 \quad (7)$$

for $S_0 = 1$ and arbitrary spin S is a solution to Eq. (6). Note that for $S = 1$ this expression reduces to $R^{(1)}(\lambda)$, Eq. (5), and for $S = \frac{1}{2}$ we reproduce^{17,21}

$$R_{S_0, \sigma}^{(1/2)}(\lambda) = (\frac{1}{2} - \lambda) + \sigma \cdot \mathbf{S}_0, \quad (8)$$

where σ are the Pauli matrices, $\mathbf{S} = \sigma/2$.

The transfer matrix $T(\lambda)$ can now be obtained using expressions (5) and (7) in Eq. (3). In order to construct the Hamiltonian describing the interaction of the chain with the impurity of spin S , it is actually only necessary to consider

$$T^*(\lambda) = \text{Tr}_0 [R_{0, m+1}^{(1)}(\lambda) R_{0, (m, s)}^{(s)}(\lambda) R_{0, m}^{(1)}(\lambda)], \quad (9)$$

since the impurity can interact only with the neighboring sites. The matrix product and the trace are evaluated in the auxiliary space V_0 and \mathcal{H}_{int} is obtained via

$$\mathcal{H}_{\text{int}} = \mathcal{H}^* - 2\mathcal{H}_{m, m+1}, \quad (10)$$

where \mathcal{H}^* is given by

$$\begin{aligned} \mathcal{H}_{\text{int}} = & \sum_{K=0}^4 \sum_{k_1, k_2=0}^2 a(K, k_1, k_2) \sum_{Q=-K}^K (K - Q \ K \ Q \ | \ K \ K \ 0 \ 0) \\ & \times \sum_{q_1=-k_1}^{k_1} \sum_{q_2=-k_2}^{k_2} (k_1 \ q_1 \ k_2 \ q_2 \ | \ k_1 \ k_2 \ K \ Q) C_Q^K(S) T_{q_1}^{k_1}(S_m) T_{q_2}^{k_2}(S_{m+1}), \end{aligned} \quad (12)$$

where the Clebsch-Gordan coefficient constraints $Q = q_1 + q_2$. The permutation invariance of the sites m and $m+1$ imposes $K + k_1 + k_2$ to be even and

$$a(K, k_2, k_1) = a(K, k_1, k_2).$$

The matrix elements of \mathcal{H}_{int} are straightforwardly obtained by means of Wigner-Eckart's theorem

$$\begin{aligned} \langle S S^* J M \ | \ \mathcal{H}_{\text{int}} \ | \ S S^* J M \rangle \\ = \sum_{K=0}^4 (-1)^{K+S^*+J+S} [(2S^*+1)(2S^{*'}+1)]^{1/2} \\ \times \begin{Bmatrix} S & S^* & J \\ S^{*'} & S & K \end{Bmatrix} \langle S \| C^K \| S \rangle \sum_{k_1, k_2=0}^2 a(K, k_1, k_2) \begin{Bmatrix} 1 & 1 & k_1 \\ 1 & 1 & k_2 \\ S^* & S^{*'} & K \end{Bmatrix} \langle 1 \| T^{k_1} \| 1 \rangle \langle 1 \| T^{k_2} \| 1 \rangle. \end{aligned} \quad (13)$$

This expression involves standard $6j$ and $9j$ symbols and $\langle || \rangle$ denotes a reduced matrix element. The coefficients $a(K, k_1, k_2)$ are now determined by comparing the matrix elements from (13) with those obtained via $T^*(\lambda)$. The values of $a(K, k_1, k_2)$ as a function of the impurity spin are given in Table I. All coefficients other than those indicated vanish. Note that $a(0, 0, 0)$ is irrelevant, since it just adds a constant to the Hamiltonian. The coefficients inserted into Eq. (12) yield the impurity interaction Hamiltonian for arbitrary impurity spin S .

Our next step consists in diagonalizing the Hamiltonian $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{int}}$. The procedure used is standard^{13,14,17,21} and we closely follow Ref. 17, such that not all the steps are presented in detail. We introduce the monodromy matrix as product of (2×2) matrices $R_{\sigma, S}^{(1/2)}$ of the type given by Eq. (8) using an auxiliary space of spin $\frac{1}{2}$ [we drop the supindex $(\frac{1}{2})$]

$$\hat{I}_\sigma(\lambda) = R_{\sigma, S_1}(\lambda) \cdots R_{\sigma, S_m}(\lambda) R_{\sigma, S_{\text{imp}}}(\lambda) R_{\sigma, S_{m+1}}(\lambda) \cdots R_{\sigma, S_N}(\lambda), \quad (14)$$

$$\mathcal{H}^* = -\frac{J}{2} T^{*-1}(0) \frac{dT^*(\lambda)}{d\lambda} \Big|_{\lambda=0}. \quad (11)$$

Since \mathcal{H}^* and $T^*(\lambda)$ commute, they can be diagonalized within the same basis of eigenstates. Since \mathcal{H}^* is invariant under the permutation of the sites m and $m+1$, the eigenstates should have well-defined parity. The total angular momentum $\mathbf{J} = \mathbf{S}_m + \mathbf{S}_{m+1} + \mathbf{S}$ and its z component are good quantum numbers of $T^*(\lambda)$. Due to parity it is convenient first to sum \mathbf{S}_m and \mathbf{S}_{m+1} to give \mathbf{S}^* , the quantum numbers for \mathbf{S}^* being 0, 1, and 2. The use of this basis makes the inversion of $T^*(0)$ straightforward and all matrix elements of and hence of \mathcal{H}_{int} are obtained.

The Hamiltonian operator \mathcal{H}_{int} is most conveniently written as linear combination of products of irreducible tensor operators for the spins \mathbf{S}_m , \mathbf{S}_{m+1} , and \mathbf{S} . We follow the definitions of Refs. 24 and 25. The irreducible tensor operators of the spin operators \mathbf{S} and \mathbf{S}_m are denoted by $C^K(S)$ and $T^k(S_m)$, respectively. Since \mathbf{S}_m and \mathbf{S}_{m+1} are spin 1 operators, k is restricted to the values 0, 1, and 2. The rank K is restricted to $K \leq 4$ if $S > 2$, to $K \leq 3$ if $S = \frac{3}{2}$, to $K \leq 2$ if $S = 1$ and $K \leq 1$ for $S = \frac{1}{2}$. The Hamiltonian is then given by

whose trace over σ is $T_\sigma(\lambda)$. Note that $S_1 = \dots = S_N = 1$, except S_{imp} which is arbitrary. $T_\sigma(\lambda)$ commutes with the transfer matrix $T(\lambda)$ defined by Eq. (3) as can be shown by using Eq. (6). Hence $T(\lambda)$ and $T_\sigma(\lambda)$ can be diagonalized simultaneously. The matrix product $I_\sigma(\lambda)$ can be written as

$$I_\sigma(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix}, \quad (15)$$

where $C(\lambda)$ and $B(\lambda)$ act as raising and lowering operators on the spin space consisting of the direct product of the spin states $S_1, \dots, S_m, S_{\text{imp}}, S_{m+1}, \dots, S_N$. The operators $A(\lambda)$, $B(\lambda)$, $C(\lambda)$, and $D(\lambda)$ obey commutation relations given in Refs. 17 and 21. Let $|\phi\rangle$ be the ferromagnetic state with maximum z component, i.e., with all spins aligned. The eigenstates of $T_\sigma = A + D$ with M spin flips are then given by

$$\psi(\lambda_1, \dots, \lambda_M) = \prod_{k=1}^M B(\lambda_k) |\phi\rangle, \quad (16)$$

where the parameters $\lambda_k = i\Lambda_k/2 + \frac{1}{2}$ satisfy

$$\left[\frac{\Lambda_j - 2Si}{\Lambda_j + 2Si} \right] \left[\frac{\Lambda_j - 2i}{\Lambda_j + 2i} \right]^N = \prod_{\substack{l=1 \\ (l \neq j)}}^M \frac{\Lambda_j - \Lambda_l - 2i}{\Lambda_j - \Lambda_l + 2i}. \quad (17)$$

Here S is the impurity spin. Within this basis also $T(\lambda)$ is diagonal with eigenvalue

$$\begin{aligned} \Lambda(\lambda; \lambda_1, \dots, \lambda_M) &= \prod_{k=1}^M \frac{\lambda - \lambda_k + \frac{3}{2}}{\lambda - \lambda_k - \frac{1}{2}} (-\lambda^2 + 3\lambda - 2)^N [\lambda - \lambda^2 + (2\lambda - 1)S - S^2] \\ &+ \prod_{k=1}^M \frac{(\lambda - \lambda_k - \frac{3}{2})(\lambda - \lambda_k + \frac{3}{2})}{(\lambda - \lambda_k - \frac{1}{2})(\lambda - \lambda_k + \frac{1}{2})} (\lambda - \lambda^2)^N [\lambda - \lambda^2 - 2 + 2S^2] \\ &+ \prod_{k=1}^M \frac{\lambda - \lambda_k - \frac{3}{2}}{\lambda - \lambda_k + \frac{1}{2}} (-\lambda - \lambda^2)^N [\lambda - \lambda^2 - (2\lambda - 1)S - S^2]. \end{aligned} \quad (18)$$

The energy eigenvalue is obtained via Eq. (2),

$$\begin{aligned} E &= -\frac{J}{2} \frac{d}{d\lambda} \ln \Lambda(\lambda; \lambda_1, \dots, \lambda_M) \Big|_{\lambda=0} \\ &= -J \sum_{j=1}^M \frac{4}{\Lambda_j^2 + 4} + \text{const}, \end{aligned} \quad (19)$$

where the parameters Λ_j are obtained from a self-consistent solution of Eq. (17). The impurity contribution to the energy arises from the first factor in Eq. (17).

The thermodynamic properties of the model are obtained in complete analogy to Ref. 17. In the thermodynamic limit the solutions of Eq. (17) lie in the complex plane and form strings length n

$$\Lambda_j^{n,\alpha} = \Lambda_j^n + i(n+1-2\alpha), \quad \alpha = 1, 2, \dots, n, \quad (20)$$

with real rapidity Λ_j^n and $n = 1, 2, \dots$. A string excitation of order n represents a bound-magnon state of n magnons. In thermal equilibrium the properties of the system at finite T and in a magnetic field H are described by the energy of these elementary string excitations $\mathcal{E}_n(\Lambda)$. It is convenient to introduce the statistical weight of these excitations,

$$\eta_n(\Lambda) = \exp[\mathcal{E}_n(\Lambda)/T], \quad (21)$$

which satisfy nonlinearly coupled integral equations

$$\ln \eta_n = G * \ln[(1 + \eta_{n-1})(1 + \eta_{n+1})] - 2\pi \frac{J}{T} \delta_{n,2} G, \quad n = 1, 2, \dots \text{ and } \eta_0 = 0. \quad (22)$$

Here the centered asterisk denotes a convolution and

$$G(\Lambda) = \left[4 \cosh \left[\frac{\pi}{2} \Lambda \right] \right]^{-1}. \quad (23)$$

These equations are completed by the asymptotic condition

$$\lim_{n \rightarrow \infty} \left[\frac{1}{n} \ln \eta_n(\Lambda) \right] = \frac{2H}{T} = 2X_0, \quad (24)$$

where H is the magnetic field. The free energy of the model can be written as

$$F = NF^{(1)} + F^{(S)}, \quad (25)$$

where

$$F^{(k)}(T, H) = F^{(k)}(0, 0) - T \int d\Lambda G(\Lambda) \ln[1 + \eta_{2k}(\Lambda)]. \quad (26)$$

Here $F^{(k)}(0, 0)$ is a constant given by

$$F^{(k)}(0, 0) = \begin{cases} -J \ln 2 & \text{for } k = \frac{1}{2}, \\ -J & \text{for } k \geq 1. \end{cases} \quad (27)$$

From Eq. (25) we have that the free energy due to the interacting impurity is $F^{(S)}(T, H)$. Here $F^{(S)}$ for $S \neq 1$ is

TABLE I. Coefficients $a(K, k_1, k_2)$ of the interaction Hamiltonian. The coefficients have the symmetry $a(K, k_2, k_1) = a(K, k_1, k_2)$ and $a(0, 0, 0)$ is irrelevant. All coefficients not listed in the table vanish.

(K, k_1, k_2)	$a(K, k_1, k_2)$	Impurity spin S
(0,1,1)	$-\sqrt{3} \frac{2S^2+2S-1}{S(S+1)}$	$S \geq \frac{1}{2}$
(0,2,2)	$-\frac{8\sqrt{5}}{15} \frac{2S^2+2S+1}{S(S+1)}$	$S \geq \frac{1}{2}$
(1,1,0) } (1,0,1) }	$\sqrt{6S(S+1)} \frac{2S^2+2S-1}{S^2(S+1)^2}$	$S \geq \frac{1}{2}$
(1,1,2) } (1,2,1) }	$-\frac{2}{5} \sqrt{15S(S+1)} \frac{S^2+S-2}{S^2(S+1)^2}$	$S \geq \frac{1}{2}$
(2,2,0) } (2,0,2) }	$\frac{8\sqrt{5}}{3} \frac{S^2+S-1}{S(S+1)}$	$S \geq 1$
(2,1,1)	$\sqrt{30} \frac{S^2+S-2}{S(S+1)}$	$S \geq 1$
(2,2,2)	$-\frac{8\sqrt{70}}{21} \frac{S^2+S-2}{S(S+1)}$	$S \geq 1$
(3,2,1) } (3,1,2) }	$-\frac{4}{3} \sqrt{210/S(S+1)}$	$S \geq \frac{3}{2}$
(4,2,2)	$\frac{32\sqrt{70}}{35}$	$S \geq 2$

not just the free energy per spin of a SU(2) Heisenberg chain of arbitrary spin S , as incorrectly claimed in Ref. 21 for the spin- $\frac{1}{2}$ Heisenberg chain with impurity. Note that the driving term of our integral equations (22) is always at $n=2$, while it is at $n=2S$ for the Heisenberg chain with arbitrary spin S .

For the spin- $\frac{1}{2}$ Heisenberg antiferromagnet with impurity we obtain, evaluating Eqs. (20) and (21) of reference 21 along the lines of the previous paragraph, for the free energy of the impurity in the limit $T \rightarrow 0$ ($J = +1$),

$$F^{(1/2)}(0, H) = -\ln 2 - \frac{H^2}{\pi^2} \left[1 - \frac{1}{2 \ln H} - \frac{\ln |\ln H|}{4 \ln^2 H} + \dots \right],$$

$S = \frac{1}{2}$

$$F^{(S)}(0, H) = -\ln 2 - 2(S - \frac{1}{2})H - SH / \ln H + \dots,$$

$S > \frac{1}{2}$ (spin- $\frac{1}{2}$ anti-ferromagnet).

Note that a spin- $\frac{1}{2}$ impurity in a spin- $\frac{1}{2}$ chain just corresponds to one more link in the chain and the corresponding zero-field susceptibility is a constant.⁴ For $S > \frac{1}{2}$ the magnetization is finite and equal to $S - \frac{1}{2}$ as $H \rightarrow 0$. We may regard the antiferromagnet as a system

with neighboring spins being antiparallel, that is, spins pairwise compensate each other giving rise to no net magnetization as $H \rightarrow 0$. An impurity of spin $S > \frac{1}{2}$ can only be compensated by one antiparallel neighbor giving rise to a net magnetization of $S - \frac{1}{2}$. We call this a partial spin compensation in analogy to a similar situation occurring for a magnetic impurity of arbitrary spin S coupled by an exchange interaction to an electron gas with spin $\frac{1}{2}$ (see, e.g., Ref. 26). A spin- $\frac{1}{2}$ Kondo impurity forms a singlet with the conduction electron spin density giving rise to no net magnetization as $H \rightarrow 0$. On the other hand, an $S > \frac{1}{2}$ Kondo impurity is only partially compensated by the conduction electron spin density (of spin $\frac{1}{2}$) yielding an impurity magnetization of $(S - \frac{1}{2})$ as $H \rightarrow 0$ at $T = 0$.

Properties of the chain without impurity, $F^{(1)}(T, H)$, have been discussed previously in the literature.^{14,15,17,27} We limit our discussion to the impurity. At high temperatures the driving term in Eq. (22) can be neglected and it is straightforward to obtain the free spin free energy^{6,17}

$$F^{(S)}(T, H) = -T \ln \{ \sinh[(2S+1)H/T] / \sinh(H/T) \}.$$

(28)

The low-temperature properties depend on the sign of the coupling constant J . For $J > 0$ (antiferromagnetic coupling) the free energy in the limit $T \rightarrow 0$ and for small fields H yields ($J = +1$)

$$F^{(1/2)}(0, H) = -\ln 2 - \frac{2}{\pi^3} H^2 |\ln H| - \frac{4}{\pi^3} H^2 + \dots,$$

$S = \frac{1}{2}$

$$F^{(1)}(0, H) = -1 - \frac{2H^2}{\pi^2} \left[1 - \frac{1}{\ln H} - \frac{\ln |\ln H|}{\ln^2 H} + \dots \right],$$

$S = 1$ (29)

$$F^{(S)}(0, H) = -1 - 2(S-1)H - 2S \frac{H}{\ln H} + \dots, \quad S > 1.$$

Hence we obtain a logarithmically diverging susceptibility for $S = \frac{1}{2}$ as $H \rightarrow 0$, a constant χ if $S = 1$ and $H \rightarrow 0$ (spin compensated impurity) and a partially compensated impurity spin if $S > 1$. As mentioned above, these results resemble those of an impurity of arbitrary spin S coupled by an exchange interaction to an electron gas with spin $\frac{1}{2}$ (Ref. 26). For ferromagnetic coupling ($J < 0$) the susceptibility diverges as $T \rightarrow 0$ according to²⁷

$$\chi^{(S)} \sim 4S \frac{|J|}{T^2} (\mathcal{L}^{-1} + \ln \mathcal{L} / \mathcal{L}^2 + \dots),$$

(30)

where $\mathcal{L} = \ln(2|J|/T)$, and the specific heat follows

$$C \sim 1.6S(2T|J|)^{1/2} + O(T).$$

(31)

In summary, we have presented an integrable model of

an impurity of arbitrary spin S interacting with a Heisenberg chain of spin 1. The Hamiltonian is $SU(2)$ invariant and the model is a generalization of both, higher-spin Heisenberg chains¹⁴⁻¹⁷ and Andrei and

Johannesson's²¹ spin- $\frac{1}{2}$ Heisenberg chain with impurity. The model is integrable by construction; we obtained its Bethe-ansatz solution and discussed some of its properties.

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