INTRODUCTION TO INTEGRABLE MANY-BODY SYSTEMS II

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This is the second part of a three-volume introductory course about integrable systems of interacting bodies. The models of interest are quantum spin chains with nearest-neighbor interactions between spin operators, in particular Heisenberg spin- $\frac{1}{2}$ models. The Ising model in a transverse field, expressible as a quadratic fermion form by using the Jordan-Wigner transformation, is the subject of Sect. 12. The derivation of the coordinate Bethe ansatz for the XXZ Heisenberg chain and the determination of its absolute ground state in various regions of the anisotropy parameter are presented in Sect. 13. The magnetic properties of the ground state are explained in Sect. 14. Sect. 15 concerns excited states and the zero-temperature thermodynamics of the XXZ model. The thermodynamics of the XXZ Heisenberg chain is derived on the basis of the string hypothesis in Sect. 16; the thermodynamic Bethe ansatz equations are analyzed in high-temperature and low-temperature limits. An alternative derivation of the thermodynamics without using strings, leading to a non-linear integral equation determining the free energy, is the subject of Sect. 17. A nontrivial application of the Quantum Inverse Scattering method to the fully anisotropic XYZ Heisenberg chain is described in Sect. 18. Sect. 19 deals with integrable cases of isotropic spin chains with an arbitrary spin.

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QUANTUM SPIN CHAINS

12 Quantum Ising chain in a transverse field

We consider quantum spin operators S_n on a closed chain of N sites n = 1, 2, ..., N, defined in Appendix A of paper I [1]. The spin components S_n^{α} ($\alpha = x, y, z$ or 1, 2, 3) fulfill the commutation relations

$$[\mathbf{S}_{n}^{\alpha}, \mathbf{S}_{m}^{\beta}] = \mathrm{i}\delta_{nm}\epsilon_{\alpha\beta\gamma}\mathbf{S}_{n}^{\gamma} \tag{12.1}$$

 $(\epsilon_{\alpha\beta\gamma})$ is the antisymmetric tensor) and the periodicity conditions $\mathbf{S}_{N+1}^{\alpha} \equiv \mathbf{S}_{1}^{\alpha}$. In the case of only nearest-neighbor interactions between spins and in the presence of an external magnetic field h along the z-axis, the most general Hamiltonian reads

$$H = \sum_{n=1}^{N} H_{n,n+1}(\mathbf{S}_n, \mathbf{S}_{n+1}) - 2h \sum_{n=1}^{N} \mathbf{S}_n^z,$$
(12.2)

where $H_{n,n+1}(\mathbf{S}_n, \mathbf{S}_{n+1})$ is a symmetric function of the spin operators. The spin- $\frac{1}{2}$ operators can be represented by Pauli spin operators on the chain as follows $\mathbf{S}_n^{\alpha} = \boldsymbol{\sigma}_n^{\alpha}/2$ and the general Heisenberg spin- $\frac{1}{2}$ Hamiltonian reads

$$H = -\frac{1}{2} \sum_{n=1}^{N} \left(J_x \sigma_n^x \sigma_{n+1}^x + J_y \sigma_n^y \sigma_{n+1}^y + J_z \sigma_n^z \sigma_{n+1}^z \right) - h \sum_{n=1}^{N} \sigma_n^z.$$
(12.3)

The spin- $\frac{1}{2}$ Heisenberg model simplifies substantially when the z-component of the coupling constant vanishes, $J_z = 0$. This so-called XY model in a transverse field was solved via a transformation to a quadratic fermion form [2, 3]. Here, we shall study its simplified version with an additional constraint $J_y = 0$, known as the quantum Ising model in a transverse field. In terms of the parameter $\lambda = J_x/2h$ and in the units of h = 1, its Hamiltonian takes the form

$$H(\lambda) = -\lambda \sum_{n=1}^{N} \boldsymbol{\sigma}_{n}^{x} \boldsymbol{\sigma}_{n+1}^{x} - \sum_{n=1}^{N} \boldsymbol{\sigma}_{n}^{z}, \qquad \boldsymbol{\sigma}_{N+1}^{\alpha} \equiv \boldsymbol{\sigma}_{1}^{\alpha}.$$
(12.4)

The case $\lambda > 0$ ($\lambda < 0$) corresponds to the ferromagnetic (antiferromagnetic) regime.

For a bipartite chain with N = even number, the chain sites can be divided into two subsets of alternating sites A and B. Due to the relation for the Pauli matrices $\sigma_n^z \sigma_n^x \sigma_n^z = -\sigma_n^x$, the unitary transformation with $U = U^{\dagger} = \prod_{n \in A} \sigma_n^z$ leaves the Hamiltonian (12.4) unchanged, except for the replacement $\lambda \to -\lambda$:

$$UH(\lambda)U^{\dagger} = H(-\lambda). \tag{12.5}$$

Thus, without any loss of generality, the real parameter λ can be chosen to take positive values.

12.1 Jordan-Wigner transformation

We consider the raising and lowering combinations of chain spin- $\frac{1}{2}$ operators

$$\mathbf{S}_{n}^{\pm} = \mathbf{S}_{n}^{x} \pm \mathbf{i}\mathbf{S}_{n}^{y}.$$
(12.6)

Since $\sigma_n^x = \mathbf{S}_n^+ + \mathbf{S}_n^-$, $\sigma_n^y = (\mathbf{S}_n^+ - \mathbf{S}_n^-)/i$ and $\sigma_n^z = 2\mathbf{S}_n^+\mathbf{S}_n^- - 1$, the Hamiltonian (12.4) can be rewritten in the form

$$H = -\lambda \sum_{n=1}^{N} \left(\mathbf{S}_{n}^{+} + \mathbf{S}_{n}^{-} \right) \left(\mathbf{S}_{n+1}^{+} + \mathbf{S}_{n+1}^{-} \right) - \sum_{n=1}^{N} \left(2\mathbf{S}_{n}^{+}\mathbf{S}_{n}^{-} - \mathbf{1} \right).$$
(12.7)

The spin chain operators $\{\mathbf{S}_n^{\pm}\}_{n=1}^N$ exhibit a "mixed statistics". They satisfy the fermion anticommutation relations on the same site

$$\{\mathbf{S}_{n}^{+}, \mathbf{S}_{n}^{-}\} = 1, \qquad (\mathbf{S}_{n}^{+})^{2} = (\mathbf{S}_{n}^{-})^{2} = 0$$
(12.8)

and the boson commutation relations for two different sites

$$[\mathbf{S}_{n}^{+}, \mathbf{S}_{n'}^{-}] = [\mathbf{S}_{n}^{+}, \mathbf{S}_{n'}^{+}] = [\mathbf{S}_{n}^{-}, \mathbf{S}_{n'}^{-}] = 0 \quad \text{for } n \neq n'.$$
(12.9)

The true annihilation operators $\{c_n\}$ and the creation operators $\{c_n^{\dagger}\}$ of spinless fermions can be constructed from the spin chain operators by using the Jordan-Wigner transformation [4]:

$$c_n = \exp\left(i\pi \sum_{m=1}^{n-1} \mathbf{S}_m^+ \mathbf{S}_m^-\right) \mathbf{S}_n^-, \qquad c_n^\dagger = \mathbf{S}_n^+ \exp\left(-i\pi \sum_{m=1}^{n-1} \mathbf{S}_m^+ \mathbf{S}_m^-\right).$$
(12.10)

To verify whether the operators $\{c_n\}$ and $\{c_n^{\dagger}\}$ indeed satisfy the fermion anticommutation relations

$$\{c_n^{\dagger}, c_{n'}\} = \delta_{nn'}, \qquad \{c_n, c_{n'}\} = \{c_n^{\dagger}, c_{n'}^{\dagger}\} = 0,$$
(12.11)

we first use the identities $\exp(\pm i\pi S_n^+ S_n^-) = -\sigma_n^z$ to rewrite the transformation (12.10) as follows

$$c_n = \prod_{m=1}^{n-1} (-\boldsymbol{\sigma}_m^z) \mathbf{S}_n^-, \qquad c_n^{\dagger} = \mathbf{S}_n^+ \prod_{m=1}^{n-1} (-\boldsymbol{\sigma}_m^z).$$
(12.12)

Since $(\sigma_n^z)^2 = 1$ and the spin operators commute for different sites, it holds

$$c_n c_n^{\dagger} = \mathbf{S}_n^- \mathbf{S}_n^+, \quad c_n^{\dagger} c_n = \mathbf{S}_n^+ \mathbf{S}_n^-, \quad (c_n)^2 = (\mathbf{S}_n^-)^2 = 0, \quad (c_n^{\dagger})^2 = (\mathbf{S}_n^+)^2 = 0, \quad (12.13)$$

i.e. the one-site anticommutation relations (12.8) are preserved by the transformation. Due to the relation $\mathbf{S}_n^+ \mathbf{S}_n^- = c_n^{\dagger} c_n$, the transformation inverse to (12.10) reads

$$\mathbf{S}_{n}^{-} = \exp\left(-\mathrm{i}\pi\sum_{m=1}^{n-1}c_{m}^{\dagger}c_{m}\right)c_{n}, \qquad \mathbf{S}_{n}^{+} = c_{n}^{\dagger}\exp\left(\mathrm{i}\pi\sum_{m=1}^{n-1}c_{m}^{\dagger}c_{m}\right).$$
(12.14)

Let us now consider two different sites $n \neq n'$, say n < n'. Using the equality $\mathbf{S}_n^- \boldsymbol{\sigma}_n^z = \mathbf{S}_n^-$, we have

$$c_n c_{n'}^{\dagger} = \mathbf{S}_n^{-} \prod_{m=n}^{n'-1} (-\boldsymbol{\sigma}_m^z) \mathbf{S}_{n'}^{+} = -\mathbf{S}_n^{-} \prod_{m=n+1}^{n'-1} (-\boldsymbol{\sigma}_m^z) \mathbf{S}_{n'}^{+}.$$
 (12.15)

On the other hand,

$$c_{n'}^{\dagger}c_n = \mathbf{S}_{n'}^{+} \prod_{m=n}^{n'-1} (-\boldsymbol{\sigma}_m^z) \mathbf{S}_n^{-} = \mathbf{S}_{n'}^{+} \prod_{m=n+1}^{n'-1} (-\boldsymbol{\sigma}_m^z) \mathbf{S}_n^{-},$$
(12.16)

where we used that $\sigma_n^z \mathbf{S}_n^- = -\mathbf{S}_n^-$. We see from the last two equations that $\{c_n, c_{n'}^{\dagger}\} = 0$. All remaining anticommutation relations in Eq. (12.11) can be verified analogously.

We want to express the original Hamiltonian (12.7) in terms of the fermion operators. The one-site terms are easy since $\mathbf{S}_n^+\mathbf{S}_n^- = c_n^\dagger c_n$. The two-site terms are less trivial. From (12.15) we find that for $n = 1, \ldots, N - 1$ it holds

$$c_{n}c_{n+1} = -\mathbf{S}_{n}^{-}\mathbf{S}_{n+1}^{-}, \quad c_{n}^{\dagger}c_{n+1}^{\dagger} = \mathbf{S}_{n}^{+}\mathbf{S}_{n+1}^{+}, c_{n}^{\dagger}c_{n+1} = \mathbf{S}_{n}^{+}\mathbf{S}_{n+1}^{-}, \qquad c_{n}c_{n+1}^{\dagger} = -\mathbf{S}_{n}^{-}\mathbf{S}_{n+1}^{+}.$$
(12.17)

For the couple of nearest-neighbor sites N and 1, we have

$$c_{N}c_{1} = (-1)^{\hat{N}_{a}}\mathbf{S}_{N}^{-}\mathbf{S}_{1}^{-}, \quad c_{N}^{\dagger}c_{1}^{\dagger} = -(-1)^{\hat{N}_{a}}\mathbf{S}_{N}^{+}\mathbf{S}_{1}^{+}, c_{N}^{\dagger}c_{1} = -(-1)^{\hat{N}_{a}}\mathbf{S}_{N}^{+}\mathbf{S}_{1}^{-}, \quad c_{N}c_{1}^{\dagger} = (-1)^{\hat{N}_{a}}\mathbf{S}_{N}^{-}\mathbf{S}_{1}^{+},$$
(12.18)

where $\hat{N}_a = \sum_{n=1}^{N} c_n^{\dagger} c_n$ is the operator of the total number of fermions. Collecting all terms, the Hamiltonian (12.7) is transformed to

$$H = -\lambda \sum_{n=1}^{N} (c_n^{\dagger} - c_n) (c_{n+1}^{\dagger} + c_{n+1}) - 2 \sum_{n=1}^{N} c_n^{\dagger} c_n + N$$
(12.19)

with the boundary conditions

$$c_{N+1} = -(-1)^{\hat{N}_a} c_1, \qquad c_{N+1}^{\dagger} = -(-1)^{\hat{N}_a} c_1^{\dagger}.$$
 (12.20)

Since the Hamiltonian (12.19) contains only bilinear combinations of fermion operators, it holds $[(-1)^{\hat{N}_a}, H] = 0$, i.e. the states with even or odd fermion numbers are preserved. Let α be the eigenvalue of the operator $(-1)^{\hat{N}_a}$: $\alpha = +1$ for even states and $\alpha = -1$ for odd states. Then, the boundary conditions (12.20) are expressed as follows

$$c_{N+1} = -\alpha c_1, \qquad c_{N+1}^{\dagger} = -\alpha c_1^{\dagger}.$$
 (12.21)

12.2 Diagonalization of the quadratic form

The Hamiltonian (12.19) is a simple quadratic form in fermion operators of type

$$H - N = \sum_{n,m=1}^{N} \left[c_n^{\dagger} A_{nm} c_m + \frac{1}{2} \left(c_n^{\dagger} B_{nm} c_m^{\dagger} + \text{h.c.} \right) \right], \qquad (12.22)$$

where

$$A_{nm} = -\lambda(\delta_{n,m-1} + \delta_{n,m+1}) - 2\delta_{nm} \pmod{N},$$
(12.23)

$$B_{nm} = -\lambda(\delta_{n,m-1} - \delta_{n,m+1}) \pmod{N}$$
(12.24)

are the elements of the real circulant matrices A, B and h.c. means hermitian conjugate. Note that the Hamiltonian is hermitian due to the symmetricity of A and the antisymmetricity of B.

We shall look for a linear transformation of the fermion operators

$$\eta_k = \sum_n \left(g_{kn} c_n + h_{kn} c_n^{\dagger} \right), \qquad \eta_k^{\dagger} = \sum_n \left(g_{kn} c_n^{\dagger} + h_{kn} c_n \right), \tag{12.25}$$

which is canonical (i.e. the operators η_k and η_k^{\dagger} also obey the fermion anticommutation rules) and simultaneously transforms the Hamiltonian (12.22) to a Hamiltonian of noninteracting spinless fermions

$$H - N = \sum_{k} \Lambda_k \eta_k^{\dagger} \eta_k + \text{const.}$$
(12.26)

If this is possible, then there must hold

$$[\eta_k, H] - \Lambda_k \eta_k = 0. \tag{12.27}$$

Substituting the transformation (12.25) into this equation and setting to zero the coefficients ahead of each operator, we arrive at a coupled set of equations for the g_{kn} and h_{kn} :

$$\Lambda_k g_{kn} = \sum_m \left(g_{km} A_{mn} - h_{km} B_{mn} \right), \quad \Lambda_k h_{kn} = \sum_m \left(g_{km} B_{mn} - h_{km} A_{mn} \right).$$
(12.28)

Introducing the linear combinations of coefficients

$$\phi_{kn} = g_{kn} + h_{kn}, \qquad \psi_{kn} = g_{kn} - h_{kn}, \tag{12.29}$$

Eqs. (12.28) are expressible as matrix equations

$$\phi_k (\mathbf{A} - \mathbf{B}) = \Lambda_k \psi_k, \qquad \psi_k (\mathbf{A} + \mathbf{B}) = \Lambda_k \phi_k.$$
 (12.30)

Eliminating either ψ_k or ϕ_k from these equations leads to the eigenvalue equations, either the one

$$\phi_k \left(\mathbf{A} - \mathbf{B} \right) \left(\mathbf{A} + \mathbf{B} \right) = \Lambda_k^2 \phi_k \tag{12.31}$$

or the one

$$\psi_k \left(\mathbf{A} + \mathbf{B} \right) \left(\mathbf{A} - \mathbf{B} \right) = \Lambda_k^2 \psi_k. \tag{12.32}$$

In the present case, we have

$$\left[(\mathbf{A} - \mathbf{B}) (\mathbf{A} + \mathbf{B}) \right]_{nm} = 4 \left[(1 + \lambda^2) \delta_{nm} + \lambda (\delta_{n,m-1} + \delta_{n,m+1}) \right] \pmod{N}.$$
(12.33)

Assuming for simplicity that the number of chain sites N is odd, the Fourier diagonalization of the circulant matrix (12.33) leads to the eigenvalues

$$\Lambda_k = 2\sqrt{1 + 2\lambda\cos k + \lambda^2}.$$
(12.34)

The values of the wave number k are determined by the boundary conditions (12.21) as follows $k = 2\pi j/N$, where j is integer (half-odd integer) for $\alpha = -1$ (+1), such that $-\pi/2 < k < \pi/2$.

Because A is symmetric and B is antisymmetric, the transposition $(\mathbf{A} + \mathbf{B})^{\mathrm{T}} = \mathbf{A} - \mathbf{B}$, and so both matrices $(\mathbf{A} - \mathbf{B})(\mathbf{A} + \mathbf{B})$ and $(\mathbf{A} + \mathbf{B})(\mathbf{A} - \mathbf{B})$ are symmetric and at least positive semi-definite. Consequently, the Λ_k 's are real and one can choose all the ϕ_k 's and ψ_k 's to be real as well as orthogonal. If the ϕ_k 's are normalized vectors, i.e. $\sum_n \phi_{kn}^2 = 1$, then the ψ_k 's are also normalized. This fact implies that

$$\sum_{n} (g_{kn}g_{k'n} + h_{kn}h_{k'n}) = \delta_{kk'}, \qquad \sum_{n} (g_{kn}h_{k'n} - h_{kn}g_{k'n}) = 0, \tag{12.35}$$

which are the necessary and sufficient conditions for $\{\eta_k\}$ and $\{\eta_k^{\dagger}\}$ to be the fermion operators.

The constant in H - N can be determined from the invariance of Tr (H - N) under the canonical transformation (12.25). From the representation (12.22), we have

$$Tr(H - N) = 2^{N-1} \sum_{n} A_{nn},$$
(12.36)

while from (12.26) we have

$$\operatorname{Tr}\left(H-N\right) = 2^{N-1} \sum_{k} \Lambda_{k} + 2^{N} \times \operatorname{const.}$$
(12.37)

The constant is thus equal to $(\sum_n A_{nn} - \sum_k \Lambda_k)/2$. We conclude that

$$H = \sum_{k} \Lambda_k \left(\eta_k^{\dagger} \eta_k - \frac{1}{2} \right), \qquad \Lambda_k = 2\sqrt{1 + 2\lambda \cos k + \lambda^2}, \tag{12.38}$$

where the sum goes over N values of the wave number k, equidistantly distributed over the interval $(-\pi/2, \pi/2)$.

12.3 Ground-state properties and thermodynamics

The ground state Ψ_0 of the transformed free-fermion Hamiltonian (12.38) is the state with no elementary excitations:

$$\eta_k |\Psi_0\rangle = \langle \Psi_0 | \eta_k^{\dagger} = 0 \qquad \text{for all } k.$$
(12.39)

The ground-state energy is given by

$$E_0 = -\frac{1}{2} \sum_k \Lambda_k. \tag{12.40}$$

In the thermodynamic limit $N \to \infty$, the sum can be replaced by an integral:

$$-\frac{E_0}{N} = \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} \sqrt{1 + \lambda^2 + 2\lambda \cos k} = \frac{2}{\pi} (1 + \lambda) E\left(\frac{\pi}{2}, \frac{2\sqrt{\lambda}}{1 + \lambda}\right),\tag{12.41}$$

where E is the elliptic integral of the second kind [5]. The ground-state energy per site is analytic in λ , except for the point $\lambda = 1$ at which the square root in the integral (12.41) vanishes for $k = \pm \pi$. The second and higher derivatives of E_0 with respect to λ diverge at $\lambda = 1$, which is the evidence of a second-order phase transition. The order parameter is $M^x = \langle \Psi_0 | \boldsymbol{\sigma}_n^x | \Psi_0 \rangle$:

$$M^{x} = \begin{cases} 0 & \text{in the disordered region } 0 \le \lambda < 1, \\ \pm M_{0}^{x} \ne 0 & \text{in the ordered region } \lambda > 1. \end{cases}$$
(12.42)

The first excited state corresponds to $k = \pm \pi$ and

$$\Lambda_{\pm\pi} = 2|1-\lambda|. \tag{12.43}$$

The gap between the ground-state energy and the excitation spectrum drops to zero, and so the ground state becomes two-fold degenerated, just at the critical point $\lambda = 1$.

Let us consider the Ising model in its critical point $\lambda = 1$, in a continuum limit of the lattice spacing $a \rightarrow 0$. In order to restore physical units in the energy-momentum relation, we measure the momentum from π as follows

$$k = \pi + ak',\tag{12.44}$$

the energy of the correct dimension is defined as

$$E(k') = \frac{\Lambda_k}{2a}.$$
(12.45)

As $a \rightarrow 0$, we have a nontrivial continuum limit of the spectrum

$$E(k') = |k'|, (12.46)$$

which corresponds to the relativistic spectrum of a massless particle. The Ising model is thus described in the vicinity of the critical point $\lambda = 1$ by a continuum field theory of free Majorana fermions [6, 7].

To derive the thermodynamics of the Ising model in a transverse field, for each momentum k we define the fermion occupation numbers $n_k = 0, 1$. For a given configuration of occupation numbers $\{n_k\}$, the energy corresponding to the Hamiltonian (12.38) is

$$E(\{n_k\}) = \sum_k \Lambda_k \left(n_k - \frac{1}{2}\right). \tag{12.47}$$

The canonical partition function at the inverse temperature $\beta = 1/T$ (in units of the Boltzmann constant $k_{\rm B} = 1$) is thus given by

$$Z_N = \sum_{\{n_k=0,1\}} \exp\left[-\beta E(\{n_k\})\right] = \prod_k 2\cosh(\beta \Lambda_k/2).$$
(12.48)

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In the thermodynamic limit $N \to \infty,$ the free energy per site f is given by

$$-\beta f = \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} \ln\left[2\cosh\left(\beta\sqrt{1+2\lambda\cos k+\lambda^2}\right)\right].$$
(12.49)

The free energy does not exhibit any singularity in λ for $T \neq 0$, i.e., arbitrarily small thermal fluctuations prevent the system from undergoing a phase transition [8].

13 XXZ Heisenberg chain: Bethe ansatz and the ground state

In the absence of the magnetic field h = 0, the Hamiltonian of the spin- $\frac{1}{2}$ Heisenberg chain is

$$H = -\frac{1}{2} \sum_{n=1}^{N} \left(J_x \boldsymbol{\sigma}_n^x \boldsymbol{\sigma}_{n+1}^x + J_y \boldsymbol{\sigma}_n^y \boldsymbol{\sigma}_{n+1}^y + J_z \boldsymbol{\sigma}_n^z \boldsymbol{\sigma}_{n+1}^z \right).$$
(13.1)

There are four basic possibilities for the coupling constants:

- $J_x = J_y = J_z = J > 0$: the isotropic ferromagnetic XXX Heisenberg chain, solved by Bethe [9] in 1931.
- $J_x = J_y = J_z = J < 0$: the isotropic antiferromagnetic XXX Heisenberg chain, the ground-state energy was obtained by Hulthén [10] in 1938 and the elementary excitations were found by de Cloizeaux & Pearson [11] in 1962.
- $(J_x = J_y = J) \neq J_z$: the XXZ Heisenberg chain, solved by Yang & Yang [12, 13] in 1966.
- $(J_x \neq J_y) \neq J_z$: the fully anisotropic XYZ Heisenberg chain, solved by Baxter [14, 15] in 1972.

13.1 Symmetries of Hamiltonian

In this part, we shall concentrate on the XXZ Heisenberg Hamiltonian

$$H(J, J_z) = -\frac{1}{2} \sum_{n=1}^{N} \left[J \left(\boldsymbol{\sigma}_n^x \boldsymbol{\sigma}_{n+1}^x + \boldsymbol{\sigma}_n^y \boldsymbol{\sigma}_{n+1}^y \right) + J_z (\boldsymbol{\sigma}_n^z \boldsymbol{\sigma}_{n+1}^z - 1) \right],$$
(13.2)

where the energy is trivially shifted by a constant. For a bipartite chain with two alternating subsets of sites A and B, the unitary transformation with $U = U^{\dagger} = \prod_{n \in A} \sigma_n^z$ leaves H unchanged, except for the replacement $J \to -J$:

$$UH(J, J_z)U^{\dagger} = H(-J, J_z).$$
 (13.3)

We can therefore restrict ourselves to the Hamiltonian

$$H(\Delta) \equiv \frac{1}{J}H(J, J_z) = -\frac{1}{2}\sum_{n=1}^{N} \left[\boldsymbol{\sigma}_n^x \boldsymbol{\sigma}_{n+1}^x + \boldsymbol{\sigma}_n^y \boldsymbol{\sigma}_{n+1}^y + \Delta(\boldsymbol{\sigma}_n^z \boldsymbol{\sigma}_{n+1}^z - 1) \right], \quad (13.4)$$

where the parameter $\Delta = J_z/J$ takes an arbitrary real value. The special cases $\Delta = 1$ and $\Delta = -1$ correspond to the ferromagnetic and antiferromagnetic isotropic Heisenberg chains, respectively.

The XXZ model exhibits another useful symmetry for N = even number of sites. Using the unitary operator $V = \exp(i\pi \sum_{n=1}^{N} n\sigma_n^z)$, we can transform H to

$$VH(\Delta)V^{\dagger} = -H(-\Delta). \tag{13.5}$$

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The energy spectra of the Hamiltonians $H(\Delta)$ and $H(-\Delta)$ are thus related by the reflection around E = 0.

With regard to the relation

$$\boldsymbol{\sigma}_{n}^{x}\boldsymbol{\sigma}_{n+1}^{x} + \boldsymbol{\sigma}_{n}^{y}\boldsymbol{\sigma}_{n+1}^{y} = 2\left(\mathbf{S}_{n}^{+}\mathbf{S}_{n+1}^{-} + \mathbf{S}_{n}^{-}\mathbf{S}_{n+1}^{+}\right)$$
(13.6)

the Hamiltonian (13.4) commutes with the total spin along the anisotropy z-axis,

$$[H(\Delta), \sum_{n=0}^{N} \mathbf{S}_{n}^{z}] = 0.$$
(13.7)

This is no longer true for the XYZ Heisenberg model.

13.2 Schrödinger equation

Since the XXZ Hamiltonian commutes with the total spin along the anisotropy axis, the solution of the Schrödinger equation

$$H(\Delta)\psi_M = E\psi_M \tag{13.8}$$

is searched as a superposition of all vectors in the Hilbert subspace with the fixed number ${\cal M}$ of down spins

$$\psi_M = \sum_{\{n\}} a(n_1, n_2, \dots, n_M) |n_1, n_2, \dots, n_M\rangle.$$
(13.9)

Here, the basis vector $|n_1, n_2, ..., n_M\rangle$ corresponds to the tensor product of M "spin-down" vectors $e^- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ put on the ordered set of chain sites

$$1 \le n_1 < n_2 < \ldots < n_M \le N \tag{13.10}$$

and (N - M) "spin-up" vectors $e^+ = {1 \choose 0}$ put on all remaining sites (see Appendix A of paper I).

To determine how the Hamiltonian (13.4) acts on a given vector $|n_1, n_2, \ldots, n_M\rangle$, we write

$$H(\Delta) = \sum_{n=1}^{N} H_{n,n+1},$$
(13.11)

where the component

$$H_{n,n+1} = -\left(\mathbf{S}_{n}^{+}\mathbf{S}_{n+1}^{-} + \mathbf{S}_{n}^{-}\mathbf{S}_{n+1}^{+}\right) + \frac{1}{2}\Delta\left(1 - \boldsymbol{\sigma}_{n}^{z}\boldsymbol{\sigma}_{n+1}^{z}\right).$$
(13.12)

acts as the unity operator on each site, except for the couple of nearest neighbors n, n+1. Since

$$\left(\mathbf{S}_{n}^{+}\mathbf{S}_{n+1}^{-}+\mathbf{S}_{n}^{-}\mathbf{S}_{n+1}^{+}\right)\begin{pmatrix}e_{n}^{\pm}\otimes e_{n+1}^{\pm}\\e_{n}^{\pm}\otimes e_{n+1}^{\mp}\end{pmatrix}=\begin{pmatrix}0\\e_{n}^{\mp}\otimes e_{n+1}^{\pm}\end{pmatrix}$$
(13.13)

and

$$\boldsymbol{\sigma}_{n}^{z}\boldsymbol{\sigma}_{n+1}^{z}\begin{pmatrix}e_{n}^{\pm}\otimes e_{n+1}^{\pm}\\e_{n}^{\pm}\otimes e_{n+1}^{\mp}\end{pmatrix} = \begin{pmatrix}e_{n}^{\pm}\otimes e_{n+1}^{\pm}\\-e_{n}^{\pm}\otimes e_{n+1}^{\mp}\end{pmatrix},$$
(13.14)

we have

$$H_{n,n+1}\begin{pmatrix} e_n^{\pm} \otimes e_{n+1}^{\pm} \\ e_n^{\pm} \otimes e_{n+1}^{\mp} \end{pmatrix} = \Delta \begin{pmatrix} 0 \\ e_n^{\pm} \otimes e_{n+1}^{\mp} \end{pmatrix} - \begin{pmatrix} 0 \\ e_n^{\mp} \otimes e_{n+1}^{\pm} \end{pmatrix}.$$
(13.15)

The whole Hamiltonian (13.11) acts on the vector $|n_1, n_2, \ldots, n_M\rangle$ as follows

$$H(\Delta)|n_1, n_2, \dots, n_M\rangle = N_{\text{anti}} \Delta |n_1, n_2, \dots, n_M\rangle - \sum_{\{n'\}} |n'_1, n'_2, \dots, n'_M\rangle.$$
(13.16)

Here, the configuration of spins down $\{n'\}$ is obtained from $\{n\}$ by the interchange of just one nearest-neighbor pair of antiparallel spins,

$$n'_1 = n_1, \quad n'_2 = n_2, \dots, \quad n'_\alpha = n_\alpha \pm 1, \dots, \quad n'_M = n_M$$
 (13.17)

and

$$N_{\text{anti}} = \sum_{\{n'\}} 1$$
 (13.18)

is the number of the nearest-neighbor antiparallel spins in the configuration $\{n\}$. Like for instance, for the spin configuration



the number of the nearest-neighbor antiparallel spins $N_{\text{anti}} = 8$ and the configuration $\{n'\}$ is generated from $\{n\}$ by interchanging either the spin down at site n_1 with its left spin-up neighbor $(n'_1 = n_1 - 1)$, or the spin at n_3 with its right neighbor $(n'_3 = n_3 + 1)$, or the spin at n_4 with one of its neighbors $(n'_4 = n_4 - 1 \text{ or } n'_4 = n_4 + 1)$, etc. The condition that ψ_M (13.9) is the eigenfunction of the Hamiltonian $H(\Delta)$ in (13.8) can be expressed as

$$Ea(\{n\}) = \sum_{\{n'\}} \left[\Delta a(\{n\}) - a(\{n'\}) \right].$$
(13.19)

This set of equations follows from the operator formula (13.16) and from the obvious equality

$$\sum_{\{n\}} a(\{n\}) \sum_{\{n'\}} |n'_1, n'_2, \dots, n'_M\rangle = \sum_{\{n\}} |n_1, n_2, \dots, n_M\rangle \sum_{\{n'\}} a(\{n'\}).$$
(13.20)

The periodic boundary conditions for the *a*-amplitudes

$$a(n_1, n_2, \dots, n_M) = a(n_2, n_3, \dots, n_M, n_1 + N),$$
 (13.21)

respect the prescribed ordering (from left to right) of sites.

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13.3 Coordinate Bethe ansatz

The derivation of the coordinate Bethe ansatz equations resembles the one for the spinless bosons with δ -function interactions on a continuous line, presented in Sect. 2.

• M = 0: The case M = 0 is trivial. The vector $|0\rangle$ with all sites in the spin-up state e^+ is the eigenvector of the Hamiltonian $H(\Delta)$ with the energy E = 0.

• M = 0: In the sector M = 1 with one spin down, Eq. (13.19) takes the form

$$Ea(n) = 2\Delta a(n) - a(n-1) - a(n+1).$$
(13.22)

The solution is the plane wave

$$a(n) = A \exp(ikn). \tag{13.23}$$

The periodicity condition a(n) = a(n+N) is equivalent to $\exp(ikN) = 1$ and the wave number k is quantized according to

$$Nk = 2\pi I, \qquad I = 0, \pm 1, \pm 2, \dots$$
 (13.24)

The number of integer *I*-values is equal to N, i.e. to the dimension of the Hilbert M = 1 subspace. The dependence of the energy E on the wave number is obtained by substituting (13.23) into the basic Eq. (13.22),

$$E = 2\left(\Delta - \cos k\right). \tag{13.25}$$

• M = 2: We have to distinguish between two cases: sites n_1 and n_2 either are or are not the nearest neighbors.

Let us start with the case when n_1 and n_2 are not the nearest neighbors, i.e. $n_2 \neq n_1 + 1$. Eq. (13.19) then reads

$$Ea(n_1, n_2) = 4\Delta a(n_1, n_2) - a(n_1 - 1, n_2) - a(n_1 + 1, n_2) -a(n_1, n_2 - 1) - a(n_1, n_2 + 1).$$
(13.26)

The general solution is

$$a(n_1, n_2) = A(12)e^{i(k_1n_1 + k_2n_2)} - A(21)e^{i(k_2n_1 + k_1n_2)},$$
(13.27)

$$E = 2(\Delta - \cos k_1) + 2(\Delta - \cos k_2), \qquad (13.28)$$

where the coefficients $A(12) \equiv A(k_1, k_2)$ and $A(21) \equiv A(k_2, k_1)$ are as-yet free.

When n_1 and n_2 are the nearest neighbors, i.e. $n_2 = n_1 + 1$, Eq. (13.19) takes the form

$$Ea(n, n+1) = 2\Delta a(n, n+1) - a(n-1, n+1) - a(n, n+2).$$
(13.29)

We look for the solution in the form (13.27), where the coefficients A(12) and A(21) will be constrained by a condition. This can be done directly by inserting the solution (13.27) into (13.29), or indirectly by extending the definition of $a(n_1, n_2)$ to identical sites $n_1 = n_2$ and putting formally $n_1 = n, n_2 = n + 1$ in Eq. (13.26):

$$Ea(n, n+1) = 4\Delta a(n, n+1) - a(n-1, n+1) - a(n+1, n+1) - a(n, n) - a(n, n+2).$$
(13.30)

The consistency of the relations (13.29) and (13.30) requires that

$$a(n+1, n+1) - 2\Delta a(n, n+1) + a(n, n) = 0.$$
(13.31)

The insertion of the solution (13.27) into this equation leads to the following relation between the *A*-coefficients:

$$\frac{A(21)}{A(12)} = \frac{e^{i(k_1+k_2)} - 2\Delta e^{ik_2} + 1}{e^{i(k_1+k_2)} - 2\Delta e^{ik_1} + 1} = \exp\left(-i\theta_{12}\right).$$
(13.32)

The phase shift $\theta_{12} \equiv \theta(k_1, k_2)$ is from the interval $\langle -\pi, \pi \rangle$. Its alternative representations read

$$\tan\left(\frac{\theta_{12}}{2}\right) = \Delta \frac{\cot(k_1/2) - \cot(k_2/2)}{(1 - \Delta)\cot(k_1/2)\cot(k_2/2) - (\Delta + 1)}$$
$$= \frac{\Delta \sin[(k_1 - k_2)/2]}{\Delta \cos[(k_1 - k_2)/2] - \cos[(k_1 + k_2)/2]}.$$
(13.33)

The phase function is antisymmetric with respect to the exchange of indices,

$$\theta_{12} = -\theta_{21},$$
 (13.34)

so that $\theta(k,k) = 0$. Setting the common prefactor to unity, the (unnormalized) A-coefficients are expressible as

$$A(12) = \exp\left(\frac{\mathrm{i}}{2}\theta_{12}\right), \qquad A(21) = \exp\left(\frac{\mathrm{i}}{2}\theta_{21}\right). \tag{13.35}$$

The wave numbers k_1 and k_2 are quantized according to the periodic boundary condition $a(n_1, n_2) = a(n_2, n_1 + N)$ as follows

$$A(12) = -A(21)e^{ik_1N}, \qquad A(21) = -A(12)e^{ik_2N}.$$
 (13.36)

These conditions can be rewritten as

$$\begin{cases} Nk_1 = 2\pi I_1 + \theta_{12} \\ Nk_2 = 2\pi I_2 + \theta_{21} \end{cases}$$
 $I_1, I_2 = \pm \frac{1}{2}, \pm \frac{3}{2}, \pm \frac{5}{2}, \dots$ (13.37)

Because I_1 and I_2 may be interchanged without affecting the solutions, we can restrict ourselves to $I_1 \leq I_2$. The wave numbers must be unequal, $k_1 \neq k_2$, in order to avoid the nullity of the wavefunction. To show that the total number of solutions for (k_1, k_2) is equal to the dimension $\binom{N}{2}$ of the Hilbert subspace M = 2 is a nontrivial task [16].

• M = 3: We have to consider all possibilities of nearest-neighbor positions for three sites $n_1 < n_2 < n_3$:

(a)
$$n_2 \neq n_1 + 1$$
, $n_3 \neq n_2 + 1$, (b) $n_2 = n_1 + 1$, $n_3 \neq n_2 + 1$,
(c) $n_2 \neq n_1 + 1$, $n_3 = n_2 + 1$, (d) $n_2 = n_1 + 1$, $n_3 = n_2 + 1$.

In the case (a), the Schrödinger Eq. (13.19) takes the form

$$Ea(n_1, n_2, n_3) = 6\Delta a(n_1, n_2, n_3) - a(n_1 - 1, n_2, n_3) - a(n_1 + 1, n_2, n_3) -a(n_1, n_2 - 1, n_3) - a(n_1, n_2 + 1, n_3) -a(n_1, n_2, n_3 - 1) - a(n_1, n_2, n_3 + 1).$$
(13.38)

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The solution is a superposition of plane waves

$$a(n_{1}, n_{2}, n_{3}) = A(123)e^{i(k_{1}n_{1}+k_{2}n_{2}+k_{3}n_{3})} - A(132)e^{i(k_{1}n_{1}+k_{3}n_{2}+k_{2}n_{3})} -A(213)e^{i(k_{2}n_{1}+k_{1}n_{2}+k_{3}n_{3})} + A(231)e^{i(k_{2}n_{1}+k_{3}n_{2}+k_{1}n_{3})} +A(312)e^{i(k_{3}n_{1}+k_{1}n_{2}+k_{2}n_{3})} - A(321)e^{i(k_{3}n_{1}+k_{2}n_{2}+k_{1}n_{3})}.$$
(13.39)

The corresponding energy is given by

$$E = 2(\Delta - \cos k_1) + 2(\Delta - \cos k_2) + 2(\Delta - \cos k_3).$$
(13.40)

In the presence of nearest-neighbor sites, we use the same trick as in the M = 2 sector. The case (b) implies

$$\frac{A(213)}{A(123)} = e^{-i\theta_{12}}, \quad \frac{A(312)}{A(132)} = e^{-i\theta_{13}}, \quad \frac{A(321)}{A(231)} = e^{-i\theta_{23}}, \tag{13.41}$$

where $\theta_{\alpha\beta} \equiv \theta(k_{\alpha}, k_{\beta})$ is the obvious generalization of the phase function to an arbitrary pair of wave numbers. The case (c) implies

$$\frac{A(132)}{A(123)} = e^{-i\theta_{23}}, \quad \frac{A(231)}{A(213)} = e^{-i\theta_{13}}, \quad \frac{A(321)}{A(312)} = e^{-i\theta_{12}}.$$
(13.42)

The case (d) does not imply any new relations. The solution of the above two equations reads

$$A(123) = \exp\left[\frac{i}{2}(\theta_{12} + \theta_{13} + \theta_{23})\right],$$

$$A(213) = \exp\left[\frac{i}{2}(\theta_{21} + \theta_{23} + \theta_{13})\right],$$

$$A(321) = \exp\left[\frac{i}{2}(\theta_{32} + \theta_{31} + \theta_{21})\right],$$

(13.43)

etc. The formal structure of A-coefficients is obvious.

The periodic boundary condition $a(n_1, n_2, n_3) = a(n_2, n_3, n_1 + N)$ implies

$$A(123) = A(231)e^{ik_1N}, \quad A(213) = A(132)e^{ik_2N}, \quad A(312) = A(123)e^{ik_3N}.$$
 (13.44)

The distinct wave numbers k_1 , k_2 and k_3 are thus quantized as follows

$$\left.\begin{array}{l}Nk_{1} = 2\pi I_{1} + \theta_{12} + \theta_{13}\\Nk_{2} = 2\pi I_{2} + \theta_{21} + \theta_{23}\\Nk_{3} = 2\pi I_{3} + \theta_{31} + \theta_{32}\end{array}\right\} \qquad I_{1}, I_{2}, I_{3} = 0, \pm 1, \pm 2, \dots$$

$$(13.45)$$

We see that the solution in the M = 3 sector is constructed with the aid of two-spin phase functions $\theta_{\alpha\beta}$. This property is maintained in higher $M = 4, 5, \ldots, N$ sectors.

• Arbitrary M: In the sector with M spins down, the coordinate Bethe ansatz has the form

$$a(n_1, n_2, \dots, n_M) = \sum_{P \in S_M} \operatorname{sign}(P) A(P) \exp\left(i \sum_{j=1}^M k_{Pj} n_j\right),$$
(13.46)

where the sum goes over all M! permutations P of numbers (1, 2, ..., M). This ansatz automatically satisfies the Schrödinger equation (13.19) when there are no nearest-neighbor sites with both spins down. The total momentum is $K = \sum_{j=1}^{M} k_j$, the corresponding energy is given by

$$E = \sum_{j=1}^{M} e(k_j), \qquad e(k) = 2(\Delta - \cos k).$$
(13.47)

When two of the sites in the sequence $n_1, n_2, ..., n_M$ are the nearest neighbors, say $n_{j+1} = n_j + 1$, the counterpart of the consistency equation (13.31) is

$$a(\dots, n_j + 1, n_j + 1, \dots) - 2\Delta a(\dots, n_j, n_j + 1, \dots) + a(\dots, n_j, n_j, \dots) = 0.$$
(13.48)

Inserting here the Bethe ansatz (13.46) leads to

$$\sum_{P \in S_M} \operatorname{sign}(P) A(P) \left[e^{i(k_{Pj} + k_{P(j+1)})} - 2\Delta e^{ik_{P(j+1)}} + 1 \right] \\ \times e^{ik_{P1}n_1 + \dots + i(k_{Pj} + k_{P(j+1)})n_j + \dots + ik_{PM}n_M} = 0.$$
(13.49)

In the summation, each permutation P is coupled with the permutation $P_{j,j+1}$ which is generated from P by the transposition of the nearest-neighbors Pj and P(j + 1), i.e. if $P = (P1, \ldots, Pj, P(j + 1), \ldots, PM)$ then $P_{j,j+1} = (P1, \ldots, P(j + 1), Pj, \ldots, PM)$. Since the corresponding A-coefficients are multiplied by the same exponential, taking into account that $sign(P) = -sign(P_{j,j+1})$ we get the condition

$$A(P) \left[e^{i(k_{Pj}+k_{P(j+1)})} - 2\Delta e^{ik_{P(j+1)}} + 1 \right] -A(P_{j,j+1}) \left[e^{i(k_{Pj}+k_{P(j+1)})} - 2\Delta e^{ik_{Pj}} + 1 \right] = 0.$$
(13.50)

Hence, $A(P_{j,j+1}) = A(P) \exp \left(-i\theta_{P_j,P(j+1)}\right)$ which leads to

$$A(P) = \exp\left(\frac{\mathrm{i}}{2} \sum_{j,l=1 \atop (j < l)}^{M} \theta_{Pj,Pl}\right).$$
(13.51)

The periodic boundary condition (13.20) is equivalent to the conditions

$$A(P) = (-1)^{M-1} A(PC) e^{ik_{P1}N} \quad \text{for arbitrary } P,$$
(13.52)

where PC is the cyclic transposition of permutation P, i.e. if P = (P1, P2, ..., PM) then PC = (P2, ..., PM, P1). Taking into account (13.51), we find

$$e^{ik_{P1}N} = (-1)^{M-1} \frac{A(P)}{A(PC)} = (-1)^{M-1} \exp\left(i\sum_{j=2}^{M} \theta_{P1,Pj}\right)$$
 for arbitrary *P*. (13.53)

Thus the wave numbers $k_1, k_2, ..., k_M$ are quantized according to the fundamental set of M coupled Bethe equations

$$Nk_{j} = 2\pi I_{j} + \sum_{\substack{l=1\\(l\neq j)}}^{M} \theta_{jl}, \qquad j = 1, 2, \dots, M,$$
(13.54)

where I_j are integers for odd M and half-integers for even M. Only solutions with distinct wave numbers are allowed to avoid the nullity of the wavefunction. The Bethe equations can be formally represented as

$$Nk = 2\pi I(k) + \sum_{k'} \theta(k, k'),$$
(13.55)

where we assumed that $\theta(k, k) = 0$.

13.4 Orbach parametrization

The phase function $\theta(k, k')$ is a nonlinear function of the wave numbers k and k' which, in general, does not depend on their difference. We shall parametrize the wave number k by the rapidity (spectral parameter) λ , $k = k(\lambda)$, in such a way that the θ -function depends on the difference of the corresponding rapidities: $\theta(k, k') = \theta(\lambda - \lambda')$. k's and λ 's are complex numbers and the parametrization $k(\lambda)$ depends on the value of the anisotropy parameter Δ [16]. We shall treat separately the regions $\Delta > 1$, $\Delta = 1$, $-1 < \Delta < 1$, $\Delta = -1$ and $\Delta < -1$.

• Ferromagnet $\Delta > 1$: We set $\Delta = \cosh \phi \ (0 < \phi < \infty)$ and consider the parametrization

$$e^{ik} = \frac{e^{i\lambda} - e^{\phi}}{e^{i\lambda + \phi} - 1} = \frac{\sin\frac{1}{2}(\lambda + i\phi)}{\sin\frac{1}{2}(\lambda - i\phi)}.$$
(13.56)

We assume that $0 < \text{Re}(k) < 2\pi$ and $-\pi < \text{Re}(\lambda) < \pi$. Within the present parametrization, the phase function (13.32) is given by

$$-e^{i\theta(k,k')} = \frac{\sin\frac{1}{2}(\lambda - \lambda' + 2i\phi)}{\sin\frac{1}{2}(\lambda - \lambda' - 2i\phi)}$$
(13.57)

and indeed depends on the difference of the rapidities. Inserting this relation into the Bethe equations (13.53), we get for each j = 1, ..., M

$$\left[\frac{\sin\frac{1}{2}(\lambda_j + \mathrm{i}\phi)}{\sin\frac{1}{2}(\lambda_j - \mathrm{i}\phi)}\right]^N = \prod_{\substack{l=1\\(l\neq j)}}^M \frac{\sin\frac{1}{2}(\lambda_j - \lambda_l + 2\mathrm{i}\phi)}{\sin\frac{1}{2}(\lambda_j - \lambda_l - 2\mathrm{i}\phi)}.$$
(13.58)

The energy is given by $E = \sum_{j=1}^{M} e(\lambda_j)$, where

$$e(\lambda) = -2C(\phi)k'(\lambda), \qquad C(\phi) \equiv \sinh \phi = \sqrt{\Delta^2 - 1}.$$
 (13.59)

The (unnormalized) coefficients (13.51) are expressible in terms of the spectral parameters as follows

$$A(P) = \prod_{j < l} \sin \frac{1}{2} \left(\lambda_{Pj} - \lambda_{Pl} + 2i\phi \right).$$
(13.60)

• Isotropic ferromagnet $\Delta = 1$: The parametrization is now given by

$$e^{ik} = \frac{\lambda + i/2}{\lambda - i/2}, \qquad -e^{i\theta(k,k')} = \frac{\lambda - \lambda' + i}{\lambda - \lambda' - i}.$$
(13.61)

The real parts of k and λ are constrained by $0 < \text{Re}(k) < 2\pi, -\infty < \text{Re}(\lambda) < \infty$. The Bethe equations read

$$\left(\frac{\lambda_j + i/2}{\lambda_j - i/2}\right)^N = \prod_{\substack{l=1\\(l\neq j)}}^M \frac{\lambda_j - \lambda_l + i}{\lambda_j - \lambda_l - i}, \qquad j = 1, 2, \dots, M.$$
(13.62)

The energy component is obtained in the form

$$e(\lambda) = \frac{1}{\lambda^2 + \frac{1}{4}} = -k'(\lambda).$$
(13.63)

The A-coefficients are given by

$$A(P) = \prod_{j < l} \left(\lambda_{Pj} - \lambda_{Pl} + \mathbf{i} \right).$$
(13.64)

• Paramagnet $|\Delta| < 1$: Let $\Delta = -\cos \gamma \ (0 < \gamma < \pi)$. The needed parametrization is

$$e^{ik} = \frac{e^{i\gamma} - e^{\lambda}}{e^{i\gamma+\lambda} - 1} = \frac{\sinh\frac{1}{2}(i\gamma-\lambda)}{\sinh\frac{1}{2}(i\gamma+\lambda)},$$
(13.65)

or, equivalently,

$$k(\lambda) = 2 \arctan\left[\frac{\tanh(\lambda/2)}{\tan(\gamma/2)}\right] \equiv \theta(\lambda|\gamma/2).$$
(13.66)

The real parts of k and λ are constrained by $-(\pi - \gamma) < \operatorname{Re}(k) < \pi - \gamma, -\infty < \operatorname{Re}(\lambda) < \infty$. The phase function is given by

$$-e^{i\theta(k,k')} = \frac{\sinh\frac{1}{2}(\lambda - \lambda' - 2i\gamma)}{\sinh\frac{1}{2}(\lambda - \lambda' + 2i\gamma)},$$
(13.67)

or

$$\theta(k,k') = 2 \arctan\left(\frac{\tanh\left[(\lambda - \lambda')/2\right]}{\tan\gamma}\right) = \theta(\lambda - \lambda'|\gamma).$$
(13.68)

The corresponding Bethe equations read

$$\left[\frac{\sinh\frac{1}{2}(i\gamma-\lambda_j)}{\sinh\frac{1}{2}(i\gamma+\lambda_j)}\right]^N = \prod_{\substack{l=1\\(l\neq j)}}^M \frac{\sinh\frac{1}{2}(\lambda_j-\lambda_l-2i\gamma)}{\sinh\frac{1}{2}(\lambda_j-\lambda_l+2i\gamma)}, \qquad j=1,2,\ldots,M,$$
(13.69)

or, equivalently,

$$N\theta(\lambda|\gamma/2) = 2\pi I(\lambda) + \sum_{\lambda'} \theta(\lambda - \lambda'|\gamma).$$
(13.70)

The energy component is found to be

$$e(\lambda) = -2C(\gamma)k'(\lambda), \qquad C(\gamma) \equiv \sin\gamma = \sqrt{1-\Delta^2}$$
(13.71)

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The A-coefficients read

$$A(P) = \prod_{j < l} \sinh \frac{1}{2} \left(\lambda_{Pj} - \lambda_{Pl} - 2i\gamma \right).$$
(13.72)

• Isotropic antiferromagnet $\Delta = -1$: The needed parametrization is

$$e^{ik} = \frac{i/2 - \lambda}{i/2 + \lambda}, \qquad k(\lambda) = 2 \arctan(2\lambda) \equiv \theta(2\lambda|0).$$
 (13.73)

The real parts of k and λ are constrained by $-\pi < \text{Re}(k) < \pi, -\infty < \text{Re}(\lambda) < \infty$. The phase function is given by

$$-e^{i\theta(k,k')} = \frac{\lambda - \lambda' - i}{\lambda - \lambda' + i}, \qquad \theta(k,k') = 2\arctan(\lambda - \lambda') = \theta(\lambda - \lambda'|0). \tag{13.74}$$

The Bethe equations take the form

$$\left(\frac{\mathrm{i}/2 - \lambda_j}{\mathrm{i}/2 + \lambda_j}\right)^N = \prod_{\substack{l=1\\(l \neq j)}}^M \frac{\lambda_j - \lambda_l - \mathrm{i}}{\lambda_j - \lambda_l + \mathrm{i}}, \qquad j = 1, 2, \dots, M,$$
(13.75)

or

$$N\theta(2\lambda|0) = 2\pi I(\lambda) + \sum_{\lambda'} \theta(\lambda - \lambda'|0).$$
(13.76)

The energy component is given by

$$e(\lambda) = -\frac{1}{\lambda^2 + \frac{1}{4}} = -k'(\lambda).$$
(13.77)

When the number of lattice sites N = even number, the Bethe Eqs. (13.62) and (13.75) for λ 's coincide while the respective energies (13.63) and (13.77) differ from one another only by the sign, which is in agreement with the equivalence of the spectra of conjugate Hamiltonians $H(\Delta)$ and $-H(-\Delta)$. The A-coefficients are given by

$$A(P) = \prod_{j < l} \left(\lambda_{Pj} - \lambda_{Pl} - \mathbf{i} \right).$$
(13.78)

• Antiferromagnet $\Delta < -1$: We set $\Delta = -\cosh \phi \ (0 < \phi < \infty).$ The needed parametrization is

$$e^{ik} = \frac{e^{\phi+i\lambda} - 1}{e^{\phi} - e^{i\lambda}} = \frac{\sin\frac{1}{2}(i\phi - \lambda)}{\sin\frac{1}{2}(i\phi + \lambda)},$$
(13.79)

i.e.

$$k(\lambda) = 2 \arctan\left[\frac{\tan(\lambda/2)}{\tanh(\phi/2)}\right] \equiv \theta(\lambda|\phi/2).$$
(13.80)

The real parts of k and λ are constrained by $-\pi < \text{Re}(k) < \pi, -\pi < \text{Re}(\lambda) < \pi$. The phase function (13.32) is given by

$$-e^{i\theta(k,k')} = \frac{\sin\frac{1}{2}(\lambda - \lambda' - 2i\phi)}{\sin\frac{1}{2}(\lambda - \lambda' + 2i\phi)},$$
(13.81)

i.e.

$$\theta(k,k') = 2 \arctan\left(\frac{\tan[(\lambda - \lambda')/2]}{\tanh\phi}\right) \equiv \theta(\lambda - \lambda'|\phi).$$
(13.82)

The Bethe equations read

$$\left[\frac{\sin\frac{1}{2}(\mathrm{i}\phi-\lambda_j)}{\sin\frac{1}{2}(\mathrm{i}\phi+\lambda_j)}\right]^N = \prod_{\substack{l=1\\(l\neq j)}}^M \frac{\sin\frac{1}{2}(\lambda_j-\lambda_l-2\mathrm{i}\phi)}{\sin\frac{1}{2}(\lambda_j-\lambda_l+2\mathrm{i}\phi)}, \qquad j=1,2,\ldots,M,$$
(13.83)

or, equivalently,

$$N\theta(\lambda|\phi/2) = 2\pi I(\lambda) + \sum_{\lambda'} \theta(\lambda - \lambda'|\phi).$$
(13.84)

The energy component is found to be

$$e(\lambda) = -2C(\phi)k'(\lambda), \qquad C(\phi) \equiv \sinh \phi = \sqrt{\Delta^2 - 1}.$$
 (13.85)

Again, for N = even number, the spectrum equivalence of the Hamiltonians $H(\Delta)$ and $-H(-\Delta)$ is reflected through the pair of equivalent Bethe Eqs. (13.58) and (13.83) and the oppositely-signed energy components (13.59) and (13.85). The A-coefficients are expressible as follows

$$A(P) = \prod_{j < l} \sin \frac{1}{2} \left(\lambda_{Pj} - \lambda_{Pl} - 2i\phi \right).$$
(13.86)

It is instructive to compare the Bethe ansatz equations obtained in this subsection with those derived in Sect. 8 by using the algebraic Bethe ansatz. The transfer matrix $T(\lambda)$ was built from the scattering matrix (8.12) with the trigonometric parametrization of the elements

$$a(\lambda) = \sin(\lambda + \eta), \quad b(\lambda) = \sin(\lambda), \quad c(\lambda) = \sin\eta, \quad d(\lambda) = 0.$$
 (13.87)

In the sector with M spins down, the eigenvalues $t(\lambda; \lambda_1, ..., \lambda_M)$ are given by Eq. (8.53), where the spectral parameters $\{\lambda_1, ..., \lambda_M\}$ are determined by the system of Bethe equations

$$\left[\frac{a(\lambda_j)}{b(\lambda_j)}\right]^N = \prod_{\substack{l=1\\(l\neq j)}}^M \frac{a(\lambda_j - \lambda_l)b(\lambda_l - \lambda_j)}{a(\lambda_l - \lambda_j)b(\lambda_j - \lambda_l)}, \qquad j = 1, 2, \dots, M.$$
(13.88)

The energy spectrum of the XXZ Hamiltonian (13.4) with $\Delta = \cos \eta$ is now expressible as follows

$$E = -\sin \eta \frac{\mathrm{d}}{\mathrm{d}\lambda} \ln t(\lambda) \Big|_{\lambda=0} + N \cos \eta$$

= $\sin \eta \sum_{j=1}^{M} \left[\cot(\lambda_j + \eta) - \cot \lambda_j \right].$ (13.89)

In the ferromagnetic region $\Delta = \cosh \phi > 1$, setting $\eta = i\phi$ in the Bethe equations (13.88), these equations coincide with (13.58) if the present spectral parameters are shifted and rescaled in the following way $\lambda \rightarrow (\lambda - i\phi)/2$. It is easy to check that the energy component deduced from (13.89) reduces after the substitution $\lambda \rightarrow (\lambda - i\phi)/2$ to the previous one (13.59). The same scenario takes place for all other values of the anisotropy parameter Δ . We conclude that the coordinate Bethe ansatz method and the QISM provide the same solution, only the definitions of the spectral parameter are different.

13.5 The ground state

In the ferromagnetic region $\Delta \ge 1$, the absolute ground state of the XXZ Heisenberg chain is trivial and corresponds to all spins up (or all spins down), i.e. M = 0 and

$$e_0 = 0, \qquad \Delta \ge 1. \tag{13.90}$$

The reference point for the region $\Delta < 1$ is $\Delta = 0$ (the XY model) at which $\theta(k, k') = 0$. The Bethe equations (13.54) then correspond to a system of free fermions,

$$Nk_j = 2\pi I_j$$
 $(j = 1, 2, ..., M),$ $E = -2\sum_{j=1}^M \cos k_j.$ (13.91)

As we know from the analysis of particles with δ -function interaction, the sequence of distinct *I*-numbers associated with the ground state in the *M*-sector reads

$$\{I_1, I_2, \dots, I_M\} = \left\{-\frac{M-1}{2}, -\frac{M-1}{2} + 1, \dots, \frac{M-1}{2}\right\}.$$
(13.92)

The absolute (global) ground state corresponds to M = N/2 for even N and $M = (N \pm 1)/2$ for odd N. Based on the continuity arguments it has been shown in Refs. [12, 13] that the same sequence of *I*-numbers determines the ground state in the whole region $\Delta < 1$. The corresponding wave numbers $k_1 < k_2 < \cdots < k_M$ are real.

In the thermodynamic limit $N \to \infty$, $M \to \infty$, with the fixed density of down spins m = M/N, the wave numbers k are distributed with a ground-state density R(k) = R(-k) between some limits -q and +q. Applying Hultén's continualization procedure explained in Sect. 2, the Bethe equations (13.55) imply an integral equation for R(k)

$$k = 2\pi F(k) + \int_{-q}^{q} \mathrm{d}k' \,\theta(k,k') R(k'), \tag{13.93}$$

where

$$F(k) \equiv \frac{I(k)}{N} = \int_0^k dk' R(k')$$
(13.94)

is the state density. To transform the kernel of the integral equation (13.93) into a difference kernel, we use the Orbach parametrization $k(\lambda)$ and introduce the density $\rho(\lambda)$ of λ 's via the relation $\rho(\lambda)d\lambda = R(k)dk$, i.e. $\rho(\lambda) = R(k)k'(\lambda)$. Since $k(\lambda) = -k(-\lambda)$, the support

 $k \in \langle -q, q \rangle$ maps onto $\lambda \in \langle -b, b \rangle$ where the limits $\pm b$ are given by $k(\pm b) = \pm q$. The integral Eq. (13.93) for R(k) can be transcribed as an integral equation for $\rho(\lambda)$,

$$k(\lambda) = 2\pi f(\lambda) + \int_{-b}^{b} d\lambda' \,\theta(\lambda - \lambda')\rho(\lambda'), \qquad (13.95)$$

where $f(\lambda) = \int_0^{\lambda} d\lambda' \rho(\lambda')$. The differentiation of this equation with respect to λ leads to the basic integral equation

$$k'(\lambda) = 2\pi\rho(\lambda) + \int_{-b}^{b} d\lambda' \,\theta'(\lambda - \lambda')\rho(\lambda'), \qquad (13.96)$$

which determines the λ -density $\rho(\lambda)$.

The density of down spins is given by

$$m = \frac{M}{N} = \int_{-b}^{b} \mathrm{d}\lambda \,\rho(\lambda). \tag{13.97}$$

This formula fixes the relationship between the limit b and the sector m. The momentum vanishes in the ground state,

$$k_0 = \frac{K_0}{N} = \int_{-b}^{b} \mathrm{d}\lambda \, k(\lambda)\rho(\lambda). \tag{13.98}$$

The ground-state energy per site is given by

$$e_0 = \frac{E_0}{N} = \int_{-b}^{b} \mathrm{d}\lambda \, e(\lambda)\rho(\lambda). \tag{13.99}$$

13.6 The absolute ground state for $\Delta < 1$

Although $\theta'(\lambda - \lambda')$ is a difference kernel, the finiteness of the limits $\pm b$ for the spectral parameter causes that the integral Eq. (13.96) is not translationally invariant and therefore not explicitly solvable. The only exception is the case when b takes its maximal value b_0 implied by the Orbach parametrization, namely $b_0 = \infty$ for $-1 \le |\Delta| < 1$ and $b_0 = \pi$ for $\Delta < -1$. In that case the operators in Eq. (13.96) are translationally invariant and the explicit solution can be obtained by using the continuous or discrete Fourier transform of the kernel. It will be seen that the choice $b = b_0$ corresponds to the *absolute* ground state with m = 1/2. We shall use the subscript 0 in $\rho_0(\lambda)$ in order to distinguish the special case $b = b_0$. Using the notation introduced in Sect. 3, Eq. (13.96) with $b = b_0$ can be written as

$$\frac{k'}{2\pi} = (I+G)\rho_0,$$
(13.100)

where G is an integral operator with kernel $G(\lambda, \lambda') = \theta'(\lambda - \lambda')/2\pi$, over the interval $-b_0 \le \lambda' \le b_0$. Introducing the resolvent operator J via the relation (I+J)(I+G) = (I+G)(I+J) = I, the formal solution of this equation is

$$\rho_0 = (I+J)\frac{k'}{2\pi}.$$
(13.101)

Denoting by \hat{G} the Fourier transform of $G(\lambda) = \theta'(\lambda)/2\pi$, the Fourier transforms of the resolvent kernel and of the λ -density are given by

$$\hat{J} = -\frac{\hat{G}}{1+\hat{G}}, \qquad \hat{\rho}_0 = \frac{1}{1+\hat{G}}\frac{\hat{k}'}{2\pi}.$$
(13.102)

• Paramagnet $-1 < \Delta = -\cos \gamma < 1$: It follows from the definition (13.68) that

$$\theta'(\lambda|\gamma) = \frac{\sin(2\gamma)}{\cosh\lambda - \cos(2\gamma)}.$$
(13.103)

Recalling that $b_0 = \infty$ in the paramagnetic region, we have

$$\hat{G}(\omega|\gamma) = \int_{-\infty}^{\infty} d\lambda \,\mathrm{e}^{-\mathrm{i}\omega\lambda} \frac{1}{2\pi} \frac{\sin(2\gamma)}{\cosh\lambda - \cos(2\gamma)} = \frac{\sinh[(\pi - 2\gamma)\omega]}{\sinh(\pi\omega)}.$$
(13.104)

From (13.66) we obtain $k'(\lambda) = \theta'(\lambda|\gamma/2)$, hence $\hat{k'}(\omega) = 2\pi \hat{G}(\omega|\gamma/2)$ and

$$\hat{\rho}_0(\omega) = \frac{\hat{G}(\omega|\gamma/2)}{1 + \hat{G}(\omega|\gamma)} = \frac{1}{2\cosh(\gamma\omega)}, \qquad \rho_0(\lambda) = \frac{1}{4\gamma} \frac{1}{\cosh(\pi\lambda/2\gamma)}.$$
(13.105)

As was anticipated, $m = \hat{\rho}_0(0) = 1/2$. The ground-state energy per site reads

$$e_0 = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \,\hat{e}(\omega)\hat{\rho}_0(\omega) = -2\sin\gamma \int_0^{\infty} \mathrm{d}\omega \,\frac{\sinh[(\pi-\gamma)\omega]}{\sinh(\pi\omega)\cosh(\gamma\omega)}.$$
(13.106)

• Isotropic antiferromagnet $\Delta = -1$: Using Eqs. (13.73)-(13.77) we find that

$$\hat{G}(\omega|0) = \int_{-\infty}^{\infty} \mathrm{d}\lambda \,\mathrm{e}^{-\mathrm{i}\omega\lambda} \frac{1}{\pi} \frac{1}{1+\lambda^2} = \mathrm{e}^{-|\omega|} \tag{13.107}$$

and

$$\hat{\rho}_0(\omega) = \frac{\hat{G}(\omega/2|0)}{1 + \hat{G}(\omega|0)} = \frac{1}{2\cosh(\omega/2)}, \qquad \rho_0(\lambda) = \frac{1}{2\cosh(\pi\lambda)}.$$
(13.108)

Consequently,

$$m = \hat{\rho}_0(0) = \frac{1}{2}, \qquad e_0 = -2 \int_{-\infty}^{\infty} \frac{d\lambda}{\cosh(\pi\lambda)(1+4\lambda^2)} = -2\ln 2.$$
 (13.109)

• Antiferromagnet $\Delta = -\cosh \phi < -1$: Since

$$\theta'(\lambda|\phi) = \frac{\sinh(2\phi)}{\cosh(2\phi) - \cos\lambda} \tag{13.110}$$

and $b_0 = \pi$, we have for integer n

$$\hat{G}(n|\phi) = \int_{-\pi}^{\pi} \mathrm{d}\lambda \,\mathrm{e}^{-\mathrm{i}n\lambda} \frac{1}{2\pi} \frac{\sinh(2\phi)}{\cosh(2\phi) - \cos\lambda} = \mathrm{e}^{-2\phi|n|}.$$
(13.111)



Fig. 13.1. The dependence of the range of k-values in the ground state on the anisotropy parameter Δ

From (13.80) we obtain $k'(\lambda) = \theta'(\lambda | \phi/2)$ which implies $\hat{k}'(s) = 2\pi \hat{G}(s | \phi/2)$. Consequently,

$$\hat{\rho}_{0}(n) = \frac{\hat{G}(n|\phi/2)}{1+\hat{G}(n|\phi)} = \frac{1}{2\cosh(\phi n)},$$

$$\rho_{0}(\lambda) = \frac{1}{4\pi} \sum_{n=-\infty}^{\infty} \frac{e^{in\lambda}}{\cosh(\phi n)} = \frac{\text{Kdn}(\text{K}\lambda/\pi, u)}{2\pi^{2}},$$
(13.112)

where

$$\mathbf{K} \equiv K(u) = \int_0^{\pi/2} \frac{\mathrm{d}\varphi}{\sqrt{1 - u^2 \sin^2 \varphi}}$$
(13.113)

is the complete elliptic integral of the first kind, whose modulus u is related to the parameter ϕ through the relation

$$\phi = \pi \frac{K(\sqrt{1-u^2})}{K(u)} \tag{13.114}$$

(for definitions of elliptic functions and integrals, see Appendix B of paper I). Thus $m=\hat{\rho}_0(0)=1/2$ and

$$e_0 = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} \hat{e}(n)\hat{\rho}_0(n) = -2\sinh\phi \sum_{n=-\infty}^{\infty} \frac{1}{1 + e^{2\phi|n|}}.$$
(13.115)

In Fig. 13.1, we show the range of k-values in the ground state as a function of the anisotropy parameter Δ .

The absolute ground-state energy is the continuous function of Δ which has singularities at the ferromagnetic ($\Delta = 1$) and antiferromagnetic ($\Delta = -1$) critical points. At $\Delta = -1$, all

its derivatives are also continuous (the phase transition is of infinite order). The ground-state energies (13.106) and (13.115) are different, however, on the real axis they coalesce ideally at $\Delta = -1$ in the sense that their values and the values of all their derivatives coincide at this point.

14 XXZ Heisenberg chain: Ground state in the presence of magnetic field

The external magnetic field h along the z axis was taken to be zero till now. In the region $\Delta < 1$, the absolute ground state corresponds to the "half-filling" with the density of down spins m = 1/2 and the density of up spins 1 - m = 1/2, hence $s^z = \sum_{n=1}^{N} \langle \mathbf{S}_n^z \rangle / N = 0$. We also looked for the *local* ground-state energy in the subspace with the fixed density of down spins

$$m = \frac{1}{2}(1-s), \qquad s = 2s^{z},$$
(14.1)

which is related in some way to the limit b of the spectral parameter λ . If m = 1/2 we have $b = b_0$, if m < 1/2 then $b < b_0$.

An alternative approach to the one of fixing m is to include the magnetic field $h \ge 0$ into the Hamiltonian and to look for the absolute ground state in the presence of this field. The contribution of the magnetic field to the energy per site (13.99) is -h(N-2M)/N, i.e.

$$e_0 = \int_{-b}^{b} \mathrm{d}\lambda \, e(\lambda)\rho(\lambda) - h\left[1 - 2\int_{-b}^{b} \mathrm{d}\lambda \, \rho(\lambda)\right]. \tag{14.2}$$

The absolute ground state corresponding to the magnetic field is determined by the minimization of this energy, which fixes a relationship between h and b, and consequently between h and m. The ground state results from the competition of two effects: The energy loss due to spin flips into the field direction and the energy gain from the spin-spin interaction part of the Hamiltonian. The present section is devoted to various aspects of this problem. General formulas are solved explicitly near the half-filling, at leading order in s.

The pioneering works in this field belong to Griffiths [17] (the calculation of the magnetization curve for the infinite antiferromagnetic XXX chain) and to Bonner and Fisher [18] (extrapolation of numerical results obtained for finite-size XXX rings).

14.1 Fundamental equation for the λ -density

We study the absolute ground state in the presence of the magnetic field h. For h = 0, the limit of λ -values b_0 and the λ -density ρ_0 (13.101) are known. For h > 0, the limit of λ -values is changed to $b < b_0$, the corresponding λ -density ρ satisfies Eq. (13.96). Let us introduce a projection operator B which restricts the limits of the integral operator from $(-b_0, b_0)$ to (-b, b), i.e., as $b \rightarrow b_0$ then $B \rightarrow I$. Using B, Eq. (13.96) can be formally written as

$$\frac{k'}{2\pi} = \rho + GB\rho. \tag{14.3}$$

The density of down spins (13.97) is expressible as

$$m = \eta^+ B \rho \tag{14.4}$$

Both quantities ρ and m depend on h only implicitly through the limit b of λ -values and so their analysis is possible without knowledge of the explicit functional dependence h(b).

Applying the operator I + J to both sides of Eq. (14.3) with G written as G = I + G - I, we obtain the fundamental integral equation for ρ :

$$\rho_0 = \rho + J(I - B)\rho. \tag{14.5}$$

Here, the projector I - B restricts the integral operator J to intervals $(-b_0, -b) \cup (b, b_0)$.

The spin-down density (14.4) can be written as

$$m \equiv \frac{1}{2}(1-s) = \eta^{+}\rho - \eta^{+}(I-B)\rho.$$
(14.6)

In view of (14.3), the first term is expressible as

$$\eta^+ \rho = \eta^+ \left(\frac{k'}{2\pi} - GB\rho\right). \tag{14.7}$$

Setting $\lambda = \infty$ in (13.66) and $\lambda = \pi$ in (13.80), we get

$$\eta^{+}k' = 2k(b_{0}) = \begin{cases} 2(\pi - \gamma) & \text{for } |\Delta| < 1, \\ 2\pi & \text{for } \Delta < -1. \end{cases}$$
(14.8)

Simultaneously, it holds

1

$$\eta^{+}GB\rho \equiv \int_{-b_{0}}^{b_{0}} \mathrm{d}\lambda \int_{-b}^{b} \mathrm{d}\lambda' \frac{\theta'(\lambda-\lambda')}{2\pi}\rho(\lambda') = \int_{-b_{0}}^{b_{0}} \mathrm{d}\lambda \frac{\theta'(\lambda)}{2\pi} \int_{-b}^{b} \mathrm{d}\lambda' \rho(\lambda')$$
$$\equiv (\eta^{+}G)(\eta^{+}B\rho) = \frac{1}{2}(1-s)\eta^{+}G.$$
(14.9)

Using Eqs. (13.104) and (13.111), we find

$$\eta^{+}G = \hat{G}(0) = \begin{cases} 1 - 2\gamma/\pi & \text{for } |\Delta| < 1, \\ 1 & \text{for } \Delta < -1. \end{cases}$$
(14.10)

Combining Eqs. (14.8)–(14.10), the formula (14.7) takes the form

$$\eta^{+}\rho = \begin{cases} (1+s)/2 - s\gamma/\pi & \text{for } |\Delta| < 1, \\ (1+s)/2 & \text{for } \Delta < -1. \end{cases}$$
(14.11)

The relation (14.6) thus becomes

$$\left(1 - \frac{\gamma}{\pi}\right)s = \eta^+ (I - B)\rho \quad \text{for } |\Delta| < 1 \tag{14.12}$$

and

$$s = \eta^+ (I - B)\rho \qquad \text{for } \Delta < -1. \tag{14.13}$$

The general formalism outlined till now is exact. Now we solve the fundamental equation (14.5) to leading order in I - B. The evaluation depends on whether $-1 \le \Delta < 1$ or $\Delta < -1$.

• **Paramagnet:** The fundamental equation is singular at half-filling for $|\Delta| < 1$ and $\Delta = -1$. Since $b_0 = \infty$, b is also very large for leading order in I - B. In the fundamental equation (14.5), the intervals $(-\infty, -b)$ and (b, ∞) are localized far away from one another and one can ignore in lowest order their mutual effect; this approximation is justified by explicitly solvable cases.

In the upper interval with large positive values of λ , the ρ_0 -density (13.105) becomes

$$\rho_0(\lambda) = \frac{1}{4\gamma} \frac{1}{\cosh\left(\frac{\pi\lambda}{2\gamma}\right)} \underset{\lambda \to \infty}{\sim} \frac{1}{2\gamma} e^{-\pi\lambda/(2\gamma)}.$$
(14.14)

Setting $\lambda = b + x \ (0 \le x < \infty)$, we have

$$\rho_0(b+x) \sim \zeta e^{-\pi x/(2\gamma)}, \qquad \zeta = \frac{1}{2\gamma} e^{-\pi b/(2\gamma)}.$$
(14.15)

 $\zeta \ll 1$ is the smallness parameter. We assume that also the unknown function ρ scales analogously, i.e.

$$\rho(b+x) \sim \zeta T(x). \tag{14.16}$$

Ignoring the effect of the lower interval integration in (14.5), T(x) is determined by the integral equation

$$T(x) + \int_0^\infty dx' J(x - x')T(x') = e^{-\pi x/2\gamma}, \qquad x \ge 0.$$
 (14.17)

This equation can be extended to x < 0 within the standard Wiener-Hopf form

$$T(x) + \int_{-\infty}^{\infty} \mathrm{d}x' \, J(x - x') T(x') = g(x) + h(x), \tag{14.18}$$

where

$$g(x) = \begin{cases} e^{-\pi x/2\gamma} & \text{for } x > 0, \\ 0 & \text{for } x < 0, \end{cases}$$
(14.19)

and

$$h(x) = \begin{cases} 0 & \text{for } x > 0, \\ \int_{-\infty}^{\infty} \mathrm{d}x' \, J(x - x') T(x') & \text{for } x < 0. \end{cases}$$
(14.20)

Since T(x) vanishes for x < 0, the Fourier transform $\hat{T}(\omega)$ is analytic in the upper half-plane $\operatorname{Im} \omega \ge 0$, denoted by Π_+ . Note that $\lim_{x\to 0^+} T(x) \ne 0$ and so T(x) exhibits the discontinuity at x = 0.

The Fourier transform of the Wiener-Hopf equation (14.18) reads

$$\left[1+\hat{J}(\omega)\right]\hat{T}(\omega) = \hat{g}(\omega) + \hat{h}(\omega).$$
(14.21)

Since $\hat{J}(\omega) = \hat{J}(-\omega)$ and $1 + \hat{J}(\omega) \neq 0$ for real ω , there exists a unique factorization [19]

$$1 + \hat{G}(\omega) = \frac{1}{1 + \hat{J}(\omega)} = F_{+}(\omega)F_{-}(\omega), \qquad -\infty < \omega < \infty.$$
(14.22)

The functions $F_+(\omega)$ and $F_-(\omega)$ are analytic and nonvanishing in the half-planes Π_+ and Π_- , respectively. The symmetry J(x) = J(-x) implies

$$F_{+}(\omega) = F_{-}(-\omega), \qquad \omega \in \Pi_{+}. \tag{14.23}$$

The normalization condition is

$$F_{+}(\omega) = 1$$
 as $|\omega| \to \infty$ in Π_{+} . (14.24)

The explicit forms of F_+ and F_- will not be needed. We only note that the relation (14.23) implies $F_+(0) = F_-(0)$ and so

$$F_{+}^{2}(0) = 1 + \hat{G}(0) = 2\left(1 - \frac{\gamma}{\pi}\right).$$
(14.25)

Using the factorization (14.22), Eq. (14.21) can be rewritten in the form

$$F_{+}^{-1}\hat{T} = F_{-}(\hat{g} + \hat{h}). \tag{14.26}$$

The lhs of this equation is analytic and bounded in Π_+ . The first term on the rhs has a decomposition

$$F_{-}\hat{g} = P_{+} \left(F_{-}\hat{g} \right) + P_{-} \left(F_{-}\hat{g} \right), \tag{14.27}$$

where the projections $P_{\pm}(F_{-}\hat{g})$, analytic in Π_{\pm} , satisfy the asymptotic conditions $P_{\pm}(F_{-}\hat{g}) = 0$ for $|\omega| \to \infty$ in Π_{\pm} . The second term on the rhs $F_{-}\hat{h}$ is analytic and bounded in Π_{-} . Thus the P_{+} projection of Eq. (14.26) yields

$$\hat{T} = F_+ P_+ \left(F_- \hat{g} \right). \tag{14.28}$$

From (14.19) we have

$$\hat{g}(\omega) = \int_0^\infty \mathrm{d}x \,\mathrm{e}^{\mathrm{i}\omega x - \pi x/2\gamma} = \frac{1}{-\mathrm{i}\omega + \pi/2\gamma}.$$
(14.29)

The decomposition (14.27) corresponds to the subtraction of the residue of \hat{g} ,

$$F_{-}(\omega)\hat{g}(\omega) = \frac{1}{-i\omega + \pi/2\gamma} \left[F_{-}(\omega) - F_{-}(-i\pi/2\gamma)\right] + \frac{F_{-}(-i\pi/2\gamma)}{-i\omega + \pi/2\gamma},$$
(14.30)

so that the first (second) term is analytic in Π_{-} (Π_{+}). The formula (14.28) then implies

$$\hat{T}(\omega) \equiv \int_0^\infty \mathrm{d}x \,\mathrm{e}^{\mathrm{i}\omega x} T(x) = \frac{1}{-\mathrm{i}\omega + \pi/2\gamma} F_+(\omega) F_-(-\mathrm{i}\pi/2\gamma). \tag{14.31}$$

Without much effort, we can express

$$\lim_{x \to 0^+} T(x) = 2 \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \hat{T}(\omega)$$
(14.32)

in terms of F_+ and F_- ; the factor 2 is due to the discontinuity of T(x) at x = 0. Since $\hat{T}(\omega)$ is analytic in Π_+ , the contour integral of $\hat{T}(\omega)$ over a closed infinite semi-circle (sc) in Π_+ is zero, i.e.

$$\int_{-\infty}^{\infty} d\omega \, \hat{T}(\omega) = -\int_{sc} d\omega \, \hat{T}(\omega) = -i\pi \lim_{|\omega| \to \infty} \omega \hat{T}(\omega).$$
(14.33)

Consequently,

$$\lim_{x \to 0^+} T(x) = \lim_{|\omega| \to \infty} (-i\omega) \hat{T}(\omega) = F_-(-i\pi/2\gamma).$$
(14.34)

A similar analysis can be accomplished for the lower interval $\lambda \in (-\infty, -b)$ in the fundamental equation (14.5). Due to the symmetry $\rho(\lambda) = \rho(-\lambda)$, we find

$$\rho(-b-x) \sim \zeta T(x). \tag{14.35}$$

The small quantity s (14.12), which measures the deviation of s^z from 0 due to the magnetic field, is expressible as

$$\left(1 - \frac{\gamma}{\pi}\right)s = \int_{b}^{\infty} \mathrm{d}\lambda\,\rho(\lambda) + \int_{-\infty}^{-b} \mathrm{d}\lambda\,\rho(\lambda) \sim 2\zeta\hat{T}(0).$$
(14.36)

Hence,

$$s = 4\zeta \frac{\gamma}{\pi - \gamma} F_{+}(0) F_{-}(-i\pi/2\gamma).$$
(14.37)

• Antiferromagnet: The formalism is much simpler for $\Delta < -1$ because the fundamental equation (14.5) is not singular at $b = \pi$. The small parameter is $\zeta = \pi - b \rightarrow 0^+$. According to the fundamental equation, the density ρ can be approximated by

$$\rho(\lambda) = \rho_0(\lambda) - \zeta \left[J(\lambda, \pi) + J(\lambda, -\pi) \right] \rho_0(\pi) + O(\zeta^2).$$
(14.38)

From (13.112) we have

$$\rho_0(\pi) = \frac{\mathrm{Kdn}(\mathrm{K}, u)}{2\pi^2} = \frac{\mathrm{K}\sqrt{1-u^2}}{2\pi^2 \mathrm{dn}(0)} = \frac{\mathrm{K}\sqrt{1-u^2}}{2\pi^2}.$$
(14.39)

Moreover, the derivative

$$\rho_0'(\pi) = \frac{\mathrm{K}^2 \mathrm{dn}'(\mathrm{K}, u)}{2\pi^3} = -\frac{\mathrm{K}^2 u^2 \mathrm{sn}(\mathrm{K}, u) \mathrm{cn}(\mathrm{K}, u)}{2\pi^3} = 0$$
(14.40)

due to the equality cn(K, u) = 0. The series expansion of s in ζ follows from Eq. (14.13):

$$s = 2\zeta\rho_0(\pi) - \zeta^2\rho_0(\pi) \left[J(\pi,\pi) + J(\pi,-\pi) + J(-\pi,\pi) + J(-\pi,-\pi)\right] + O(\zeta^3).$$
(14.41)

14.2 Formula for magnetic field

Our next task is to find the relation between the magnetic field h and the λ -limit b which minimizes the energy (14.2).

We change infinitesimally the range of λ 's, $b \to b + \Delta b$. The λ -distribution $\rho(\lambda)$, defined by Eq. (13.96), is changed to $\rho(\lambda) + \Delta \rho(\lambda)$. The equation for $\Delta \rho(\lambda)$ reads

$$\Delta\rho(\lambda) + \int_{-b}^{b} \mathrm{d}\lambda' \,\frac{\theta'(\lambda-\lambda')}{2\pi} \Delta\rho(\lambda') = -\frac{1}{2\pi} \left[\theta'(\lambda-b) + \theta'(\lambda+b)\right]\rho(b)\Delta b. \tag{14.42}$$

The change of the energy becomes

$$\Delta e_0 = \int_{-b}^{b} \mathrm{d}\lambda \, e(\lambda) \Delta \rho(\lambda) + 2e(b)\rho(b)\Delta b + 2h \left[\int_{-b}^{b} \mathrm{d}\lambda \, \Delta \rho(\lambda) + 2\rho(b)\Delta b \right], \quad (14.43)$$

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where we used the symmetries $\rho(\lambda) = \rho(-\lambda)$ and $e(\lambda) = e(-\lambda)$. Let us consider the function $C(\lambda) = -\Delta\rho(\lambda)/[2\rho(b)\Delta b]$. According to (14.42), it is expressible as the sum

$$C(\lambda) = C_{+}(\lambda) + C_{-}(\lambda), \qquad (14.44)$$

where $C_{\pm}(\lambda)$ obey the integral equations

$$C_{\pm}(\lambda) + \int_{-b}^{b} \mathrm{d}\lambda' \,\frac{\theta'(\lambda - \lambda')}{2\pi} C_{\pm}(\lambda') = \frac{1}{4\pi} \theta'(\lambda \pm b). \tag{14.45}$$

Since the relation $\theta(\lambda) = -\theta(-\lambda)$ implies $\theta'(\lambda) = \theta'(-\lambda)$, it holds $C_{\pm}(\lambda) = C_{\mp}(-\lambda)$. Introducing $D(\lambda) \equiv 2C_{-}(\lambda)$, which satisfies the equation

$$D(\lambda) + \int_{-b}^{b} \mathrm{d}\lambda' \,\frac{\theta'(\lambda - \lambda')}{2\pi} D(\lambda') = \frac{1}{2\pi} \theta'(\lambda - b),\tag{14.46}$$

the energy change is expressible as

$$\frac{\Delta e_0}{4\rho(b)\Delta b} = \frac{1}{2} \left[e(b) - \int_{-b}^{b} \mathrm{d}\lambda \, e(\lambda) D(\lambda) \right] + h \left[1 - \int_{-b}^{b} \mathrm{d}\lambda \, D(\lambda) \right]. \tag{14.47}$$

Since

$$e = -2Ck' = -4\pi C \left(\rho + GB\rho\right), \tag{14.48}$$

it can be readily shown that

$$e(b) - \int_{-b}^{b} \mathrm{d}\lambda \, e(\lambda) D(\lambda) = -4\pi C \rho(b). \tag{14.49}$$

Defining $L(\lambda)$ as the solution of the equation

$$\eta = L + GBL,\tag{14.50}$$

we find that

$$1 - \int_{-b}^{b} \mathrm{d}\lambda \, D(\lambda) = L(b). \tag{14.51}$$

The consideration of Eqs. (14.49) and (14.51) in (14.47) gives

$$\frac{\Delta e_0}{4\rho(b)\Delta b} = -2\pi C\rho(b) + hL(b). \tag{14.52}$$

The extremal condition for the energy minimum is $\Delta e_0/\Delta b = 0$. The magnetic field is thus given by

$$h = \frac{2\pi C\rho(b)}{L(b)}.\tag{14.53}$$

The relationship between the field and the magnetization is mediated by the parameter b. This parameter varies from 0 to b_0 .

The case b = 0 is identified with m = 0 ($s^z = 1/2$), i.e. all spins up. For b = 0 we see from (13.96) that $\rho(\lambda) = k'(\lambda)/2\pi$ and from (14.50) that $L(\lambda) = 1$. The corresponding magnetic field (14.53) has the unique form in the whole region $\Delta < 1$:

$$h(b=0) \equiv h_u = Ck'(0) = 1 - \Delta.$$
(14.54)

Above this "upper" magnetic field, the ground state is ferromagnetic with all spins up.

As we know, the case $b = b_0$ corresponds to m = 1/2 ($s^z = 0$). The projection operator B becomes I at this point. Eq. (14.50) for $L_0(\lambda)$ and its solution read

$$\eta = L_0 + GL_0, \qquad L_0 = (I+J)\eta. \tag{14.55}$$

The function $L_0(\lambda)$ is therefore constant, equal to

$$L_0 = 1 + \hat{J}(0) = \frac{1}{1 + \hat{G}(0)} = \begin{cases} \pi/2(\pi - \gamma) & \text{for } |\Delta| < 1, \\ 1/2 & \text{for } \Delta < -1. \end{cases}$$
(14.56)

The analysis of the point $b = b_0$ and of its neighborhood depends on whether $|\Delta| < 1$ or $\Delta < -1$.

• **Paramagnet:** Since $\rho_0(\infty) = 0$, we have trivially from (14.53) that

$$h(b=\infty) \equiv h_l = 0 \tag{14.57}$$

for the "lower" magnetic field in the paramagnetic field.

If b is close to b_0 we find the field h(b) to leading order in I - B by using the Wiener-Hopf technique. From (14.16) and (14.34), $\rho(b)$ can be expressed as

$$\rho(b) \sim \zeta \lim_{x \to 0^+} T(x) = \zeta F_{-}(-i\pi/2\gamma).$$
(14.58)

To determine L(b), we write formally G = I + G - I in (14.50) and multiply both side by (I + J), to arrive at

$$L_0 = L + J(I - B)L. (14.59)$$

In the upper interval $\lambda = b + x$ ($0 \le x < \infty$), we set

$$L(b+x) \sim L_0 U(x),$$
 (14.60)

where U(x) obeys the Wiener-Hopf integral equation

$$U(x) + \int_0^\infty \mathrm{d}x \, J(x - x') U(x') = 1. \tag{14.61}$$

Since the kernel is J(x - x'), we can use the factorization (14.22) by the same functions F_+ and F_- . Simple computation leads to

$$\hat{U}(\omega) = \frac{1}{-i(\omega + i0)} F_{+}(\omega) F_{-}(0).$$
(14.62)

Consequently,

$$\lim_{x \to 0^+} U(x) = \lim_{|\omega| \to \infty} (-i\omega) \hat{U}(\omega) = F_-(0) = F_+(0).$$
(14.63)



Fig. 14.1. Phase diagram of the XXZ Heisenberg chain in the magnetic field h

From (14.60) we conclude that

$$L(b) \sim \frac{\pi}{2(\pi - \gamma)} F_{+}(0).$$
 (14.64)

Substituting this L(b) together with $\rho(b)$ from (14.58) into the formula (14.53), we finally obtain

$$h = 4\zeta(\pi - \gamma)\sin\gamma \frac{F_{-}(-i\pi/2\gamma)}{F_{+}(0)}.$$
(14.65)

To obtain the relationship between h and s, we divide Eqs. (14.65) and (14.37) and apply the relation (14.25) for $F_{+}^{2}(0)$, with the result

$$\frac{h}{s} = \frac{\pi^2}{2} \left(1 - \frac{\gamma}{\pi} \right) \frac{\sin \gamma}{\gamma}.$$
(14.66)

• Antiferromagnet: The lower field is nonzero in the antiferromagnetic region,

$$h(b = \pi) \equiv h_l(\phi) = 4\pi C \rho_0(\pi) = \frac{2\sinh\phi}{\pi} K \sqrt{1 - u^2}.$$
(14.67)

For $-h_l(\phi) < h < h_l(\phi)$, the magnetic field has no effect on the system which is in the antiferromagnetic phase with $s^z = 0$. The two-fold degenerate ground state is characterized by a staggered magnetization on the alternating sublattices. A finite magnetic field $h_l(\phi)$ is required to destroy the antiferromagnetic order and to make the total magnetization nonzero. The phase diagram is pictured in Fig.14.1. It has the reflection $h \rightarrow -h$ symmetry, the ferromagnetic ground state for negative values of the field corresponds to $s^z = -1/2$, i.e. all spins down. Note that the magnetic field considered as the function of the magnetization, $h(s^z)$, has a discontinuity at $s^z = 0$, $h(\pm 0) = \pm h_l$. To determine the small- ζ expansion of *h*, we find from (14.38) that

$$\rho(b) = \rho_0(\pi) \left\{ 1 - \zeta \left[J(\pi, \pi) + J(\pi, -\pi) \right] \right\} + O(\zeta^2)$$
(14.68)

and from (14.59) that

$$L(b) = L_0 \left\{ 1 - \zeta \left[J(\pi, \pi) + J(\pi, -\pi) \right] \right\} + O(\zeta^2).$$
(14.69)

Consequently,

$$h = h_l + O(\zeta^2). \tag{14.70}$$

14.3 Ground state energy near half-filling

Now we investigate the change of the ground state energy caused by a small magnetic field h.

The ground state energy (14.2) is first rewritten as

$$e_0 = e^+ B\rho - hs = e^+ \rho - e^+ (I - B)\rho - hs.$$
(14.71)

With regard to the fundamental equation (14.5), this expression is equivalent to

$$e_0 + hs = e^+ \rho_0 - e^+ (I+J)(I-B)\rho = e^+ \rho_0 - \rho^+ (I-B)(I+J)e.$$
(14.72)

Using the relation e = -2Ck' and Eq. (13.101), the energy change due to the magnetic field $\Delta e_0 \equiv e_0 - e^+ \rho_0$ is given by

$$\Delta e_0 = 4\pi C \rho^+ (I - B) \rho_0 - hs = 4\pi C \rho_0^+ (I - B) \rho - hs.$$
(14.73)

• **Paramagnet:** Taking into account relations (14.15) and (14.16) for the upper interval and the analogous ones for the lower interval, we write

$$\Delta e_0 = 4\pi \sin \gamma \, \zeta^2 2 \int_0^\infty \mathrm{d}x \, \mathrm{e}^{-\pi x/2\gamma} T(x) - hs = 8\pi \sin \gamma \, \zeta^2 \hat{T}(\mathrm{i}\pi/2\gamma) - hs.$$
(14.74)

The formal solution (14.31) tells us that

$$\hat{T}(i\pi/2\gamma) = \frac{\gamma}{\pi} F_{+}(i\pi/2\gamma) F_{-}(-i\pi/2\gamma) = \frac{\gamma}{\pi} F_{-}^{2}(-i\pi/2\gamma).$$
(14.75)

At the same time, the multiplication of (14.37) and (14.65) yields

$$hs = 16\gamma \sin \gamma \, \zeta^2 F_-^2(-i\pi/2\gamma). \tag{14.76}$$

In view of the last two equations, Eq. (14.74) becomes

$$\Delta e_0 = -\frac{1}{2}hs = -\frac{1}{\pi(\pi - \gamma)}\frac{\gamma}{\sin\gamma}h^2.$$
(14.77)

We see that the energy decrease -hs originating from a direct interaction with the magnetic field is only partially compensated by the amount hs/2 from the spin-spin interaction part. Note that the explicit forms of the functions $F_{+}(\omega)$ and $F_{-}(\omega)$ were not needed to the considered order. To lowest order, the magnetic susceptibility at zero magnetic field is given by

$$\chi = -\frac{\partial^2}{\partial h^2} e_0 = \frac{2}{\pi(\pi - \gamma)} \frac{\gamma}{\sin\gamma}.$$
(14.78)

• Antiferromagnet: With respect to equations (14.38), (14.41) and (14.70), the energy change is

$$\Delta e_0 = 4\pi C \left(\int_b^{\pi} \mathrm{d}\lambda + \int_{-\pi}^{-b} \mathrm{d}\lambda \right) \rho_0(\lambda)\rho(\lambda) - hs = O(\zeta^3).$$
(14.79)

15 XXZ Heisenberg chain: Excited states

15.1 Strings

Although the general analysis of the Bethe ansatz equations is complicated for a finite number of sites N, it simplifies substantially in the thermodynamic limit $N \to \infty$. When the number of down spins M is finite, the Bethe equations exhibit in the spectral-parameter space the complex string bound states which play an essential role in the finite-temperature thermodynamics. The strings are low-lying excitations from the ground state in the ferromagnetic region $\Delta \ge 1$. To explain their origin and nature, we start with the relatively simple case of the isotropic ferromagnet region $\Delta > 1$ and finally consider the paramagnetic region $|\Delta| < 1$.

• $\Delta = 1$: In the sector M = 1, the Bethe equation (13.62) reads

$$e^{ikN} = \left(\frac{\lambda + i/2}{\lambda - i/2}\right)^N = 1.$$
(15.1)

In the limit $N \to \infty$, the wave numbers k cover continuously the whole interval $(0, 2\pi)$ and the rapidities λ cover the real axis. The excitations of this type are called magnons. The energy of a magnon with the wave number k is

$$e(k) = 2(1 - \cos k). \tag{15.2}$$

In the sector with M = 2 spin downs, the Bethe equations read

$$\left(\frac{\lambda_1 + i/2}{\lambda_1 - i/2}\right)^N = \frac{\lambda_1 - \lambda_2 + i}{\lambda_1 - \lambda_2 - i}, \qquad \left(\frac{\lambda_2 + i/2}{\lambda_2 - i/2}\right)^N = \frac{\lambda_2 - \lambda_1 + i}{\lambda_2 - \lambda_1 - i}.$$
(15.3)

Let us first study *real* solutions and denote $(\lambda_1 - \lambda_2 + i)/(\lambda_1 - \lambda_2 - i) = \exp(i\varphi), \varphi \in \mathbb{R}$. Then,

$$e^{ik_1N} = e^{i\varphi}, \qquad e^{ik_2N} = e^{-i\varphi}.$$
(15.4)

In the limit $N \to \infty$, k_1 and k_2 once again cover continuously the interval $(0, 2\pi)$. We have the state of two independent magnons with the total energy

$$e(k_1) + e(k_2) = 4 \left[1 - \cos\left(\frac{k_1 + k_2}{2}\right) \cos\left(\frac{k_1 - k_2}{2}\right) \right].$$
(15.5)

The system of two equations (15.3) exhibits also complex solutions

$$\lambda_1 = u_1 + iv_1, \qquad \lambda_2 = u_2 + iv_2,$$
(15.6)

where u's and v's are real numbers. Comparing the modulus of lhs and rhs of the first equation in (15.3), we obtain the condition

$$\left[\frac{u_1^2 + (v_1 - 1/2)^2}{u_1^2 + (v_1 + 1/2)^2}\right]^N = \frac{(u_1 - u_2)^2 + (v_1 - v_2 - 1)^2}{(u_1 - u_2)^2 + (v_1 - v_2 + 1)^2}.$$
(15.7)

Let us assume that $v_1 > 0$. As $N \to \infty$, the lhs of (15.7) goes exponentially to 0, so the rhs implies

$$u_1 = u_2 = u, \qquad v_1 - v_2 = 1.$$
 (15.8)
The multiplication of two equations in (15.3) leads to the condition

$$\left[\frac{u + i(v_1 + 1/2)}{u + i(v_1 - 3/2)}\right]^N = 1,$$
(15.9)

from which, in the limit $N \to \infty$, $v_1 = 1/2$ and $u \in \mathbb{R}$. The consequent M = 2 string solution

$$\lambda_1 = u + \frac{i}{2}, \qquad \lambda_2 = u - \frac{i}{2}$$
 (15.10)

is the bound state of two magnons with the total momentum

$$K = k_1 + k_2 = \frac{1}{i} \ln\left(\frac{u+i}{u-i}\right)$$
(15.11)

and the energy

$$E_2 = \frac{1}{\lambda_1^2 + 1/4} + \frac{1}{\lambda_2^2 + 1/4} = \frac{2}{u^2 + 1} = 1 - \cos K.$$
(15.12)

For the given values of wave numbers k_1 and k_2 , this energy is always lower than the sum of energies for two independent magnons (15.5).

We would like to document that the string (15.10) is in fact the only complex solution for rapidities which ensures the normalizability of the wavefunction in the limit of an infinite chain. The wavefunction (13.46) in the M = 2 sector, with the A-coefficients given by (13.64), is proportional to

$$a(n_1, n_2) \propto \left[\left(\frac{\lambda_1 + i/2}{\lambda_1 - i/2} \right) \left(\frac{\lambda_2 + i/2}{\lambda_2 - i/2} \right) \right]^{n_1} \left\{ (\lambda_1 - \lambda_2 + i) \left(\frac{\lambda_2 + i/2}{\lambda_2 - i/2} \right)^{n_2 - n_1} - (\lambda_2 - \lambda_1 + i) \left(\frac{\lambda_1 + i/2}{\lambda_1 - i/2} \right)^{n_2 - n_1} \right\}.$$
(15.13)

Since the site label n_1 can be arbitrarily large in the limit $N \to \infty$, the normalizability of $a(n_1, n_2)$ requires that

$$\left| \left(\frac{\lambda_1 + i/2}{\lambda_1 - i/2} \right) \left(\frac{\lambda_2 + i/2}{\lambda_2 - i/2} \right) \right| = 1.$$
(15.14)

Under this condition, in order to ensure that the wavefunction is regular at asymptotically large distances $n_2 - n_1 \rightarrow \infty$, one of the terms on the rhs of (15.13) must disappear. For the present string solution (15.10) with $\text{Im}(\lambda_1) > \text{Im}(\lambda_2)$, the condition (15.14) is equivalent to the one

$$\left|\frac{u+\mathrm{i}}{u-\mathrm{i}}\right| = 1,\tag{15.15}$$

i.e. u is real. Consequently,

$$\left|\frac{\lambda_1 + i/2}{\lambda_1 - i/2}\right| = \left|\frac{u + i}{u}\right| > 1, \qquad \left|\frac{\lambda_2 + i/2}{\lambda_2 - i/2}\right| = \left|\frac{u}{u - i}\right| < 1.$$
(15.16)

The "dangerous" term on the rhs of Eq. (15.13) is the second one and its prefactor vanishes for the string (15.10), as it should be. Since the nonzero amplitude of the wavefunction (15.13) decays to 0 as $n_2 - n_1 \rightarrow \infty$, the resulting two-magnon state is the bound state.

In the limit $N \to \infty$, the string solutions of the Bethe equations exist in each sector with M spins down [9, 20]. Let us introduce the notation

$$z_j \equiv e^{ik_j} = \frac{\lambda_j + i/2}{\lambda_j - i/2} \qquad j = 1, 2, \dots, M$$
(15.17)

and assume that $\text{Im}(k_1) \ge \text{Im}(k_2) \ge \ldots \ge \text{Im}(k_M)$. The wave function (13.46) with M down spins at site positions $n_1 < n_2 < \ldots < n_M$ is then rewritten as

$$a(n_1, n_2, \dots, n_M) = (z_1 z_2 \dots z_M)^{n_1} \sum_{P \in S_M} \operatorname{sign}(P) A(P) \times \prod_{j=1}^{M-1} \left(\prod_{l=j+1}^M z_{Pl} \right)^{n_{j+1}-n_j},$$
(15.18)

where

$$A(P) = \prod_{j < l} (\lambda_{Pj} - \lambda_{Pl} + \mathbf{i}).$$
(15.19)

The normalizability condition of the wave function is consistent with the requirement that

$$|z_1 z_2 \dots z_M| = 1 \tag{15.20}$$

and that A(P) = 0 if one of the products $|\prod_{l=j+1}^{M} z_{Pl}| (j = 1, 2, ..., M - 1)$ is greater than 1, i.e.

$$A(I) \neq 0, \qquad A(P) = 0 \quad \text{if } P \neq I.$$
 (15.21)

Simultaneously, there must hold 1

$$\left| \prod_{l=j+1}^{M} z_l \right| < 1 \qquad \text{for all } j = 1, 2, \dots, M-1$$
(15.22)

in order to ensure that the term P = I vanishes for large distances $n_2 - n_1, n_3 - n_2, \ldots$ $n_M - n_{M-1}$. All these conditions are satisfied only if the rapidities form an M-string,

$$\lambda_j = u + \frac{i}{2}(M + 1 - 2j), \qquad j = 1, 2, \dots, M.$$
 (15.23)

From the condition

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$$|z_1 z_2 \dots z_M| = \left| \frac{u + iM/2}{u - iM/2} \right| = 1$$
 (15.24)

we conclude that u must be real. Since the inequality

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$$1 > \left| \prod_{l=j+1}^{M} z_l \right| = \left| \frac{u + i(M - 2j)/2}{u - iM/2} \right|$$
(15.25)

is satisfied for all j = 1, 2, ..., M - 1, strings of arbitrary length M are allowed for $\Delta = 1$. Each string of type (15.23) is an entity characterized by the total momentum

$$K = \frac{1}{i} \sum_{j=1}^{M} \ln\left(\frac{\lambda_j + i/2}{\lambda_j - i/2}\right) = \frac{1}{i} \ln\left(\frac{u + iM/2}{u - iM/2}\right)$$
(15.26)

and the energy

$$E_M = \sum_{j=1}^M \frac{1}{\lambda_j^2 + 1/4} = \frac{M}{u^2 + M^2/4}.$$
(15.27)

The dispersion relation for the M-string reads

$$E_M = \frac{2}{M} \left(1 - \cos K \right).$$
(15.28)

• $\Delta > 1$: The Orbach parametrization for the ferromagnetic region $\Delta = \cosh \phi \ (\phi > 0)$ is expressed by Eqs. (13.56)-(13.60). Introducing

$$z_j \equiv e^{ik_j} = \frac{\sin\frac{1}{2}(\lambda_j + i\phi)}{\sin\frac{1}{2}(\lambda_j - i\phi)} \qquad j = 1, 2, \dots, M,$$
(15.29)

the wave function in the sector of M down spins takes the form (15.18) with the coefficients

$$A(P) = \prod_{j < l} \sin \frac{1}{2} \left(\lambda_{Pj} - \lambda_{Pl} + 2i\phi \right).$$
(15.30)

The normalizability conditions (15.20) and (15.21) are satisfied only if

$$\lambda_j = u + i\phi (M + 1 - 2j), \qquad j = 1, 2, \dots, M.$$
 (15.31)

From the requirement

$$|z_1 z_2 \dots z_M| = \left| \frac{\sin \frac{1}{2} (u + i\phi M)}{\sin \frac{1}{2} (u - i\phi M)} \right| = 1$$
(15.32)

we see that u must be real and from the interval $(-\pi, \pi)$. Since the inequality

$$1 > \left| \prod_{l=j+1}^{M} z_l \right| = \frac{\sin \frac{1}{2} [u + i\phi(M - 2j)]}{\sin \frac{1}{2} (u - i\phi M)} = \sqrt{\frac{\cosh[\phi(M - 2j)] - \cos u}{\cosh(\phi M) - \cos u}}$$
(15.33)

is satisfied for all j = 1, 2, ..., M - 1, strings of arbitrary length M are possible in the ferromagnetic region.

The total momentum and the energy of the M-string are given by

$$K = \frac{1}{i} \sum_{j=1}^{M} \ln \left[\frac{\sin \frac{1}{2} (\lambda_j + i\phi)}{\sin \frac{1}{2} (\lambda_j - i\phi)} \right] = \frac{1}{i} \ln \left[\frac{\sin \frac{1}{2} (u + i\phi M)}{\sin \frac{1}{2} (u - i\phi M)} \right],$$
(15.34)

$$E_M = \sum_{j=1}^M \frac{2\sinh^2 \phi}{\cosh \phi - \cos \lambda_j} = \frac{2\sinh \phi \sinh(\phi M)}{\cosh(\phi M) - \cos u}.$$
(15.35)

Since

$$\cos K = \frac{1 - \cos u \cosh(\phi M)}{\cosh(\phi M) - \cos u},\tag{15.36}$$

the dispersion relation reads

$$E_M = \frac{2\sinh\phi}{\sinh(\phi M)} \left[\cosh(\phi M) - \cos K\right].$$
(15.37)

The lowest energy state in the sector with M down spins is the M string with zero total momentum K = 0 and the energy $E_{0,M} = 2 \sinh \phi \tanh(\phi M/2)$.

• $|\Delta| < 1$: The Orbach parametrization for the paramagnetic region $\Delta = -\cos\gamma \ (0 < \gamma < \pi)$ is expressed by Eqs. (13.65)–(13.72). Introducing

$$z_j \equiv e^{ik_j} = \frac{\sinh \frac{1}{2}(i\gamma - \lambda_j)}{\sin \frac{1}{2}(i\gamma + \lambda_j)} \qquad j = 1, 2, \dots, M,$$
(15.38)

the wave function for M down spins takes the form (15.18) with the coefficients

$$A(P) = \prod_{j < l} \sinh \frac{1}{2} \left(\lambda_{Pj} - \lambda_{Pl} - 2i\gamma \right).$$
(15.39)

The normalizability conditions (15.20) and (15.21) are satisfied for two kinds of strings: strings with "parity" v = 1 have the center on the real axis ($u \in \mathbb{R}$)

$$\lambda_j = u + i\gamma (M + 1 - 2j), \qquad j = 1, 2, \dots, M$$
(15.40)

and strings with parity v = -1 are centered on the $i\pi$ axis

$$\lambda_j = u + i\pi + i\gamma (M + 1 - 2j), \qquad j = 1, 2, \dots, M.$$
 (15.41)

For a given value of the anisotropy parameter γ and the parity v, there exist strong restrictions on possible lengths M of the strings [23, 24]. The normalizability conditions (15.22) for the v = 1 string

$$1 > \left| \prod_{l=j+1}^{M} z_l \right| = \left| \frac{\sinh \frac{1}{2} \left[i\gamma(2j-M) - u \right]}{\sinh \frac{1}{2} \left(i\gamma M + u \right)} \right| = \sqrt{\frac{\cosh u - \cos \gamma(M-2j)}{\cosh u - \cos(\gamma M)}}$$
(15.42)

are equivalent to the inequalities

$$\cos(\gamma M) < \cos\gamma(M-2j)$$
 for $j = 1, 2, ..., M-1$ $(v = 1)$. (15.43)

The normalizability conditions (15.22) for the v = -1 string

$$1 > \left| \prod_{l=j+1}^{M} z_l \right| = \left| \frac{\cosh \frac{1}{2} \left[i\gamma(2j - M) - u \right]}{\cosh \frac{1}{2} \left(i\gamma M + u \right)} \right| = \sqrt{\frac{\cosh u + \cos \gamma(M - 2j)}{\cosh u + \cos(\gamma M)}}$$
(15.44)

are equivalent to the inequalities

$$\cos(\gamma M) > \cos\gamma(M-2j)$$
 for $j = 1, 2, ..., M-1$ $(v = -1)$. (15.45)

The conditions (15.43) and (15.45) can be cast into the one

$$0 < 2v \sin \gamma (M - j) \sin(\gamma j) \qquad j = 1, 2, \dots M - 1.$$
(15.46)

The M-string has the total momentum and the energy

$$K = \frac{1}{i} \ln \frac{\sinh \frac{1}{2} \left[i\gamma M - u - i(1-v)\pi/2 \right]}{\sinh \frac{1}{2} \left[i\gamma M + u + i(1-v)\pi/2 \right]},$$
(15.47)

$$E_M = -\frac{2\sin\gamma\sin(\gamma M)}{v\cosh u - \cos(\gamma M)}.$$
(15.48)

The dispersion relation reads

$$E_M = -\frac{2\sin\gamma}{\sin(\gamma M)} \left[\cos(\gamma M) + \cos K\right].$$
(15.49)

The momentum is restricted to the region

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$$|K| < \pi - \left(\gamma M - \pi \left[\frac{\gamma M}{\pi}\right]\right) \qquad \text{for } v = 1 \tag{15.50}$$

and to the region

$$\pi \ge |K| > \pi - \left(\gamma M - \pi \left[\frac{\gamma M}{\pi}\right]\right) \quad \text{for } v = -1.$$
 (15.51)

We recall that the described strings determine the thermodynamics, but are not low-lying excitations from the ground state in the paramagnetic region.

• $\Delta \leq -1$: Since the energy spectra of the Hamiltonians $H(\Delta)$ and $H(-\Delta)$ are related by the reflection around E = 0, the string solutions for $\Delta = -1$ and $\Delta < -1$ are basically the same as their ferromagnetic counterparts (15.23) and (15.31), respectively, without any restrictions on the length M of the strings. The fundamental difference is that these are not low-lying excitations from the ground state in the antiferromagnetic region.

15.2 Response of the ground state to a perturbation

To obtain low-lying excitations from the ground state for $\Delta < 1$, we study in analogy with Sect. 3.1 the response of the ground state to an external phase perturbation $\phi(\lambda)$. This perturbation causes the shift of λ 's by small amounts $\Delta(\lambda)$ of order 1/N, $\lambda \to \lambda + \Delta(\lambda)$. The Bethe equations (13.55), written in terms of rapidities as follows

$$Nk(\lambda) = 2\pi I(\lambda) + \sum_{\lambda'} \theta(\lambda - \lambda'), \qquad (15.52)$$

are modified by the perturbation to

$$N[k(\lambda) + k'(\lambda)\Delta(\lambda)] = 2\pi I(\lambda) + \sum_{\lambda'} \theta[\lambda + \Delta(\lambda) - \lambda' - \Delta(\lambda')] + \phi[\lambda + \Delta(\lambda)].$$
(15.53)

Expanding to first order and subtracting Eq. (15.52) leads to

$$Nk'(\lambda)\Delta(\lambda) = \sum_{\lambda'} \theta'(\lambda - \lambda') \left[\Delta(\lambda) - \Delta(\lambda')\right] + \phi(\lambda).$$
(15.54)

Replacing the summation by an integral and using Eq. (13.96), we obtain

$$2\pi N\rho(\lambda)\Delta(\lambda) + N \int_{-b}^{b} d\lambda' \,\theta'(\lambda - \lambda')\rho(\lambda')\Delta(\lambda') = \phi(\lambda).$$
(15.55)

Defining the function $\omega(\lambda) = \rho(\lambda)\Delta(\lambda)N$, the response of the ground state to the perturbation ϕ is described by the equation

$$(I+G)\omega = \frac{\phi}{2\pi}.$$
(15.56)

Its formal solution is

$$\omega = (I+J)\frac{\phi}{2\pi}.\tag{15.57}$$

The change of the momentum due to the perturbation $\phi(\lambda)$, $\Delta K = K$ ($K_0 = 0$), is given by the sum of k's shifts as follows

$$K = \sum_{\lambda} k'(\lambda)\Delta(\lambda) \to N \int_{-b}^{b} d\lambda \,\rho(\lambda)k'(\lambda)\Delta(\lambda)$$
$$= \int_{-b}^{b} d\lambda \,k'(\lambda)\omega(\lambda) \equiv (k')^{+}\omega.$$
(15.58)

Using the formal expression (15.57) for ω and the symmetricity of the kernel $I(\lambda, \lambda') + J(\lambda, \lambda')$, this expression becomes

$$K = (k')^{+} (I+J) \frac{\phi}{2\pi} = \phi^{+} (I+J) \frac{k'}{2\pi} = \phi^{+} \rho.$$
(15.59)

Since

$$E = \sum_{\lambda} e[\lambda + \Delta(\lambda)] \sim \sum_{\lambda} e(\lambda) + \sum_{\lambda} e'(\lambda)\Delta(\lambda), \qquad (15.60)$$

the change of the ground-state energy is

$$\Delta E = \sum_{\lambda} e'(\lambda) \Delta(\lambda) \to N \int_{-b}^{b} d\lambda \,\rho(\lambda) e'(\lambda) \Delta(\lambda) = \int_{-b}^{b} d\lambda \,e'(\lambda) \omega(\lambda)$$
$$\equiv (e')^{+} \omega = (e')^{+} (I+J) \frac{\phi}{2\pi} = \phi^{+} (I+J) \frac{e'}{2\pi}.$$
(15.61)

For $|\lambda| \leq b$, we define the function $\epsilon(\lambda)$ as the solution of the integral equation

$$(I+G)\epsilon = e - \mu, \tag{15.62}$$

where the constant μ is chosen in such a way that $\epsilon(\pm b) = 0$. The formal solution is

$$\epsilon = (I+J)e - (I+J)\mu. \tag{15.63}$$

Equation (15.62) can be differentiated with respect to λ . Taking into account that G is a difference kernel, the integration by parts leads to

$$(I+G)\epsilon' = e',$$
 i.e. $\epsilon' = (I+J)e'.$ (15.64)

In terms of ϵ , the formula (15.61) can be rewritten as

$$\Delta E = \phi^+ \frac{\epsilon'}{2\pi} = -\epsilon^+ \frac{\phi'}{2\pi}.$$
(15.65)

The ground-state energy per site (13.107) can be reexpressed as follows

$$\frac{E_0}{N} = e^+ R = e^+ (I+J) \frac{k'}{2\pi} = (k')^+ (I+J) \frac{e}{2\pi} = (k')^+ \frac{\epsilon + (I+J)\mu}{2\pi}$$
$$= (k')^+ \frac{\epsilon}{2\pi} + \mu \eta^+ (I+J) \frac{k'}{2\pi} = (k')^+ \frac{\epsilon}{2\pi} + \mu \frac{M}{N}.$$
(15.66)

For a chain of N sites and M spins down, $E_0 = -PN + \mu M$, where $P = -(k')^+ \epsilon/(2\pi)$ is the pressure and μ is the chemical potential of down spins which are interpreted as "particles".

15.3 Low-lying excitations

By continuity in Δ from the free-fermion point $\Delta = 0$ to the whole region $\Delta < 1$, the excitations from the ground state are of type I ("particle excitations") and of type II ("hole excitations"), see Sect. 3.3. The basic distribution functions $\rho(\lambda)$ and $\epsilon(\lambda)$ are defined by the integral equations (13.96) and (15.62), respectively, only for $|\lambda| \leq b$. We shall need an analytic continuations of these integral equations to extend the definition of these functions to all real λ , including $|\lambda| > b$:

$$\rho(\lambda) = \frac{k'(\lambda)}{2\pi} - \int_{-b}^{b} \mathrm{d}\lambda' \,\frac{\theta'(\lambda - \lambda')}{2\pi} \rho(\lambda'), \qquad -\infty < \lambda < \infty; \tag{15.67}$$

$$\epsilon(\lambda) = e(\lambda) - \mu - \int_{-b}^{b} d\lambda' \frac{\theta'(\lambda - \lambda')}{2\pi} \epsilon(\lambda'), \qquad -\infty < \lambda < \infty.$$
(15.68)

A "particle excitation" is created by taking a particle from $\lambda = b$ to $\lambda_p > b$ (or from -b to $\lambda_p < -b$), respecting $\Delta M = 0$. This generates in the Bethe equations (15.52) the phase perturbation

$$\phi(\lambda) = \theta(\lambda - \lambda_p) - \theta(\lambda - b). \tag{15.69}$$

According to the response equation (15.65), we find

$$\Delta E(\lambda_p) = e(\lambda_p) - e(b) - \epsilon^+ \frac{\phi'}{2\pi} = \epsilon(\lambda_p), \qquad (15.70)$$

i.e. $\epsilon(\lambda)$ is the excitation energy. Using (15.59), the momentum of the particle excitation is given by

$$K(\lambda_p) = k(\lambda_p) - k(b) + \phi^+ \rho = 2\pi \left[f(\lambda_p) - f(b) \right].$$
(15.71)

Here, $f(\lambda)$ is the analytic continuation of the state density, defined by the integral Eq. (13.95), to $|\lambda| > b$:

$$f(\lambda) = \frac{k(\lambda)}{2\pi} - \int_{-b}^{b} d\lambda' \,\frac{\theta(\lambda - \lambda')}{2\pi} \rho(\lambda'), \qquad -\infty < \lambda < \infty.$$
(15.72)

Creating a "hole excitation" by taking a particle from λ_h ($0 < \lambda_h < b$) to $\lambda = b$, the perturbation in the Bethe equations becomes $\phi(\lambda) = -\theta(\lambda - \lambda_h) + \theta(\lambda - b)$. The energy and momentum changes are now

$$\Delta E(\lambda_h) = -e(\lambda_h) + e(b) - \epsilon^+ \frac{\phi'}{2\pi} = -\epsilon(\lambda_h), \qquad (15.73)$$

$$K(\lambda_h) = -k(\lambda_h) + k(b) + \phi^+ \rho = 2\pi \left[f(b) - f(\lambda_h) \right].$$
(15.74)

Since the excited energy changes $\Delta E(\lambda_p)$ and $\Delta E(\lambda_h)$ are positive, it must hold that $\epsilon(\lambda) < 0$ for $|\lambda| < b$ and $\epsilon(\lambda) > 0$ for $|\lambda| > b$.

The group velocity

$$v(\lambda) = \frac{\mathrm{d}(\Delta E)}{\mathrm{d}K} = \frac{\Delta E'}{K'} = \frac{\epsilon'(\lambda)}{2\pi\rho(\lambda)}$$
(15.75)

has the same form for both particle and hole types of excitations. The velocity of sound is given by $v_s = v(b)$.

The formalism simplifies substantially for the absolute ground state characterized by m = 1/2 and $b = b_0$. In this case, the unity function $\eta(\lambda) \equiv 1$ is an eigenvector of the integral equation $(I+G)\eta = [1+\hat{G}(0)]\eta$. Recalling that $e(\lambda) = -2Ck'(\lambda)$ and comparing Eq. (15.67) with Eq. (15.68), we obtain

$$\epsilon_0(\lambda) = -4\pi C \rho_0(\lambda) - \frac{\mu}{1 + \hat{G}(0)}.$$
(15.76)

Since $\epsilon_0(\pm b_0) = 0$, the chemical potential is given by

$$\mu = -4\pi C[1 + G(0)]\rho_0(b_0). \tag{15.77}$$

• **Paramagnet:** Since $b_0 = \infty$ and $\rho_0(b_0) = 0$, we have $\mu = 0$. In view of the relation $2\pi f_0(\lambda) = \arctan[\sinh(\pi\lambda/2\gamma)]$, the momentum of the hole excitation is

$$K(\lambda) = \frac{\pi}{2} - \arctan[\sinh(\pi\lambda/2\gamma)].$$
(15.78)

The hole-excitation energy is

$$\Delta E(\lambda) = 4\pi \sin \gamma \,\rho_0(\lambda) = \frac{\pi \sin \gamma}{\gamma} \frac{1}{\cosh(\pi \lambda/2\gamma)}.$$
(15.79)

$$\Delta E(K) = \frac{\pi \sin \gamma}{\gamma} |\sin K|.$$
(15.80)

The excitation spectrum is gapless. The velocity of sound is

$$v_s = \frac{\mathrm{d}\Delta E(K)}{\mathrm{d}K}\Big|_{K=0} = \frac{\pi \sin \gamma}{\gamma}.$$
(15.81)

The are no particle excitations in the paramagnetic region.

• Isotropic antiferromagnet: Also for this case $b_0 = \infty$ and $\mu = 0$. Since $2\pi f_0(\lambda) = \arctan[\sinh(\pi\lambda)]$, the momentum of the hole excitation is

$$K(\lambda) = \frac{\pi}{2} - \arctan[\sinh(\pi\lambda)].$$
(15.82)

The corresponding energy is

$$\Delta E(\lambda) = 2\pi\rho_0(\lambda) = \frac{\pi}{\cosh(\pi\lambda)}.$$
(15.83)

The dispersion relation takes the form

$$\Delta E(K) = \pi |\sin K| \tag{15.84}$$

and $v_s = \pi$.

• Antiferromagnet: Now $b_0 = \pi$, $\hat{G}(0) = 1$ and the chemical potential is given by

$$|\mu| = \mu_l(\phi) = 2h_l(\phi), \tag{15.85}$$

where h_l (14.67) is the smallest magnetic field which destroys the antiferromagnetic order; the factor 2 is due to the equivalence $\mu \leftrightarrow 2h$. As before, there is a discontinuity of the chemical potential $\mu(s^z)$ across $s^z = 0$, $\mu(\pm 0) = \pm \mu_l$. The ambiguity of the chemical potential in the M = N/2 sector causes some problems in interpreting the above excitation formalism. In order to remain in this sector, we add a hole and a particle which repeal each other (since they belong to different parts of the doubly degenerate antiferromagnetic ground state). This is manifested by the presence of an energy gap μ_l between the ground state and low-lying excitations. For example, in the case of hole-type excitations, the formula (15.73) should be modified as follows

$$\Delta E(\lambda) = \mu_l - \epsilon(\lambda) = \frac{\mu_l}{2} \left[1 + \frac{1}{\sqrt{1 - u^2}} \operatorname{dn}\left(\frac{\mathrm{K}\lambda}{\pi}, u\right) \right].$$
(15.86)

Since $2\pi f_0(\lambda) = \arcsin[\operatorname{sn}(K\lambda/\pi, u)]$, the momentum of the hole excitation is given by

$$K(\lambda) = \frac{\pi}{2} - \arcsin\left[\sin\left(\frac{K\lambda}{\pi}, u\right)\right].$$
(15.87)

The dispersion relation thus reads

$$\Delta E(K) = \frac{\mu_l}{2} \left(1 + \frac{\sqrt{1 - u^2 \cos^2 K}}{\sqrt{1 - u^2}} \right).$$
(15.88)

The velocity of sound is $v_s = 0$, i.e. the medium is incompressible. In the phase diagram in Fig. 14.1, the ground state has an energy gap in white (ferromagnetic and antiferromagnetic) regions and the spectrum becomes gapless in the shaded region.

16 XXX Heisenberg chain: Thermodynamics with strings

16.1 Thermodynamic Bethe ansatz

In this part, we derive the finite-temperature thermodynamics for the isotropic Heisenberg chain, defined by the Hamiltonian

$$H = -\frac{J}{2} \sum_{n=1}^{N} (\vec{\sigma}_n \cdot \vec{\sigma}_{n+1} - 1) - h \sum_{n=1}^{N} \sigma_n^z, \qquad \vec{\sigma}_{N+1} \equiv \vec{\sigma}_1.$$
(16.1)

Here, J > 0 (J < 0) corresponds to the ferromagnetic (antiferromagnetic) case and the magnetic field $h \ge 0$. The derivation of the thermodynamics is based on the string hypothesis and the particle-hole formalism [25–28], developed in Sects. 4 and 11.

Following the Orbach parametrization (13.58)–(13.61), the energy eigenvalues in the sector with $M \leq N/2$ spins down are given by

$$E = J \sum_{\alpha=1}^{M} \frac{1}{\lambda_{\alpha}^2 + 1/4} - h(N - 2M),$$
(16.2)

where the rapidities $\{\lambda_{\alpha}\}_{\alpha=1}^{M}$ satisfy the set of M coupled Bethe equations

$$\left(\frac{\lambda_{\alpha} + i/2}{\lambda_{\alpha} - i/2}\right)^{N} = -\prod_{\beta=1}^{M} \frac{\lambda_{\alpha} - \lambda_{\beta} + i}{\lambda_{\alpha} - \lambda_{\beta} - i}, \qquad \alpha = 1, 2, \dots, M.$$
(16.3)

Introducing the symbol

$$e_n(\lambda) \equiv \frac{\lambda + in/2}{\lambda - in/2},$$
(16.4)

the Bethe equations can be written in a compact form

$$[e_1(\lambda_\alpha)]^N = -\prod_{\beta=1}^M e_2(\lambda_\alpha - \lambda_\beta).$$
(16.5)

In the thermodynamic limit $N \to \infty$, rapidity solutions organize themselves into a collection of strings of various lengths $n = 1, 2, \ldots$ Like in (15.23), the rapidities of a given string are distributed equidistantly and symmetrically around the real axis. A particular solution of the Bethe equations (16.5) is characterized by a set of non-negative integers $\{M_n\}_{n=1}^{\infty}$, where M_n is the number of strings of length n. Since the total number of rapidities is equal to M, the numbers of strings are constrained by $\sum_{n=1}^{\infty} nM_n = M$. For each n, there are M_n distinct real centers λ_{α}^n ($\alpha = 1, \ldots, M_n$). The string is the set of complex rapidities

$$\lambda_{\alpha}^{(n,r)} = \lambda_{\alpha}^{n} + i\left(\frac{n+1}{2} - r\right), \qquad r = 1, 2, \dots, n.$$
 (16.6)

In the string format, the Bethe equations (16.5) take the form

. .

$$\left[e_1(\lambda_{\alpha}^{(n,r)})\right]^N = -\prod_{m=1}^{\infty} \prod_{\beta=1}^{M_m} \prod_{s=1}^m e_2(\lambda_{\alpha}^{(n,r)} - \lambda_{\beta}^{(m,s)}).$$
(16.7)

Applying the product operator $\prod_{r=1}^{n}$ to both sides of Eq. (16.7), we obtain a coupled set of equations for the real centers λ_{α}^{n} of the strings:

$$[e_n(\lambda_\alpha^n)]^N = (-1)^n \prod_{m=1}^\infty \prod_{\beta=1}^{M_m} E_{nm}(\lambda_\alpha^n - \lambda_\beta^m),$$
(16.8)

where

$$E_{nm}(\lambda) \equiv e_{|n-m|}(\lambda)e_{|n-m|+2}^{2}(\lambda)\cdots e_{n+m-2}^{2}(\lambda)e_{n+m}(\lambda).$$
(16.9)

To derive this result, we used the relations [25, 26]

$$\prod_{r=1}^{n} e_m(\lambda_{\alpha}^{(n,r)}) = \prod_{l=1}^{\min(n,m)} e_{n+m+1-2l}(\lambda_{\alpha}^n)$$
(16.10)

and

$$\prod_{r=1}^{n} \prod_{s=1}^{m} e_2(\lambda_{\alpha}^{(n,r)} - \lambda_{\beta}^{(m,s)}) = E_{nm}(\lambda_{\alpha}^n - \lambda_{\beta}^m).$$
(16.11)

For any real λ and n > 0, it holds

$$\ln e_n(\lambda) = i \left[\pi - \theta_n(\lambda) \right] \pmod{2\pi i}, \qquad \theta_n(\lambda) \equiv 2 \arctan\left(\frac{2\lambda}{n}\right). \tag{16.12}$$

Taking the logarithm of Eq. (16.8), we obtain

$$N\theta_n(\lambda_\alpha^n) = 2\pi I_\alpha^n + \sum_{m=1}^\infty \sum_{\beta=1}^{M_m} \Theta_{nm}(\lambda_\alpha^n - \lambda_\beta^m), \tag{16.13}$$

where

$$\Theta_{nm}(\lambda) = (1 - \delta_{nm})\theta_{|n-m|}(\lambda) + 2\theta_{|n-m|+2}(\lambda) + \dots + 2\theta_{n+m-2}(\lambda) + \theta_{n+m}(\lambda).$$
(16.14)

Here, I_{α}^n are integers or half-integers constrained by $-I_{\max}^n \leq I_{\alpha}^n \leq I_{\max}^n$; the value of the bound I_{\max}^n is found from the condition

$$\lambda_{\alpha}^{n} \to \infty \quad \text{for} \quad I_{\alpha}^{n} = I_{\max}^{n} + \frac{1}{2},$$
(16.15)

i.e., the string momentum has to reach its maximum value just one elementary step beyond I_{\max}^n . Since $\theta_n(\lambda \to \infty) = \pi$ (n > 0), this condition is equivalent to the constraint

$$|I_{\alpha}^{n}| \leq \frac{1}{2} \left(N - 1 - \sum_{m=1}^{\infty} t_{nm} M_{m} \right), \qquad t_{nm} = 2\min(n,m) - \delta_{nm}.$$
(16.16)

For every set of admissible quantum numbers $\{I_{\alpha}^n\}$, such that $I_{\alpha}^n \neq I_{\beta}^n$ for $\alpha \neq \beta$, there exists a unique Bethe set of rapidities $\{\lambda_{\alpha}^n\}$, no two of which are identical. Such solutions are called

"particle rapidities". Counting the number of rapidity sets for all M = 0, 1, ..., N [25], the total number of multiplet states was found to be 2^N , so they constitute a complete set.

Now we adopt the "hole" concept. Given a set of particle quantum numbers $\{I_{\alpha}^{n}\}$, we define the set of the quantum numbers $\{\tilde{I}_{\alpha}^{n}\}$ to be the admissible values from the interval (16.16) which are omitted in $\{I_{\alpha}^{n}\}$. The corresponding hole rapidities $\{\tilde{\lambda}_{\alpha}^{n}\}$ satisfy the counterpart of Eq. (16.13):

$$N\theta_n(\tilde{\lambda}^n_\alpha) = 2\pi \tilde{I}^n_\alpha + \sum_{m=1}^{\infty} \sum_{\beta=1}^{M_m} \Theta_{nm}(\tilde{\lambda}^n_\alpha - \lambda^m_\beta).$$
(16.17)

In terms of the function

$$h^{n}(\lambda) \equiv \frac{1}{2\pi} \left[\theta_{n}(\lambda) - \frac{1}{N} \sum_{m=1}^{\infty} \sum_{\beta=1}^{M_{m}} \Theta_{nm}(\lambda - \lambda_{\beta}^{m}) \right], \qquad (16.18)$$

the particle and hole quantum numbers are given by

$$I_{\alpha}^{n} = Nh^{n}(\lambda_{\alpha}^{n}), \qquad \tilde{I}_{\alpha}^{n} = Nh^{n}(\tilde{\lambda}_{\alpha}^{n}).$$
(16.19)

In the thermodynamic limit $N \to \infty$, the distributions of the real *n*-string particle centers $\{\lambda_{\alpha}^n\}$ and hole centers $\{\tilde{\lambda}_{\alpha}^n\}$ are characterized by the respective densities $\rho_n(\lambda)$ and $\tilde{\rho}_n(\lambda)$, such that

$$N\rho_n(\lambda)d\lambda = \text{number of } \lambda^n \text{'s in } d\lambda,$$

$$N\tilde{\rho}_n(\lambda)d\lambda = \text{number of } \tilde{\lambda}^n \text{'s in } d\lambda.$$
(16.20)

There exists a constraint between the particle and hole densities. According to Eq. (16.19),

$$N \left[\rho_n(\lambda) + \tilde{\rho}_n(\lambda) \right] d\lambda = \text{number of } \lambda^n \text{'s and } \lambda^n \text{'s in } d\lambda$$
$$= N \left[h^n(\lambda + d\lambda) - h^n(\lambda) \right] = N dh^n.$$
(16.21)

Consequently,

$$\rho_n(\lambda) + \tilde{\rho}_n(\lambda) = \frac{\mathrm{d}h^n}{\mathrm{d}\lambda}.$$
(16.22)

Combining this relation with Eq. (16.18), the replacement

$$\sum_{\beta=1}^{M_m} \dots \to N \int_{-\infty}^{\infty} \mathrm{d}\lambda' \,\rho_m(\lambda') \dots \tag{16.23}$$

leads to

$$\rho_n(\lambda) + \tilde{\rho}_n(\lambda) = \frac{1}{2\pi} \frac{\mathrm{d}\theta_n(\lambda)}{\mathrm{d}\lambda} - \sum_{m=1}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}\lambda' \, \frac{1}{2\pi} \frac{\mathrm{d}\Theta_{nm}(\lambda - \lambda')}{\mathrm{d}\lambda} \rho_m(\lambda'). \tag{16.24}$$

This set of equations can be rewritten in the form

$$\tilde{\rho}_n + \sum_{m=1}^{\infty} A_{nm} * \rho_m = a_n \qquad (n = 1, 2, ...),$$
(16.25)

where

$$a_n(\lambda) = \frac{1}{2\pi} \frac{\mathrm{d}\theta_n(\lambda)}{\mathrm{d}\lambda} = \frac{1}{2\pi} \frac{n}{\lambda^2 + (n^2/4)}$$
(16.26)

and

$$A_{nm}(\lambda) = \delta(\lambda)\delta_{nm} + \frac{1}{2\pi} \frac{\mathrm{d}\Theta_{nm}(\lambda)}{\mathrm{d}\lambda} = \delta(\lambda)\delta_{nm} + (1 - \delta_{nm})a_{|n-m|}(\lambda) + 2a_{|n-m|+2}(\lambda) + \dots + 2a_{n+m-2}(\lambda) + a_{n+m}(\lambda).$$
(16.27)

The Fourier transforms of $a_n(\lambda)$ and $A_{nm}(\lambda)$ read

$$\hat{a}_n(\omega) = e^{-n|\omega|/2}, \qquad \hat{A}_{nm}(\omega) = \left(\coth\frac{|\omega|}{2}\right) \left[e^{-|n-m||\omega|/2} - e^{-(n+m)|\omega|/2}\right].$$
 (16.28)

We introduce the "inverse" function $A_{nm}^{-1}(\lambda)$ by

$$\sum_{n'=1}^{\infty} \left(A_{nn'}^{-1} * A_{n'm} \right) (\lambda) = \delta(\lambda) \delta_{nm}.$$
(16.29)

Using the convolution theorem, we get

$$\hat{A}_{nm}^{-1}(\omega) = \delta_{nm} - \hat{s}(\omega) \left(\delta_{n,m+1} + \delta_{n,m-1} \right),$$
(16.30)

where

$$\hat{s}(\omega) = \frac{1}{2\cosh(\omega/2)}, \qquad s(\lambda) = \frac{1}{2\cosh(\pi\lambda)}.$$
(16.31)

The energy of an *n*-string for J = 1 is given in Eq. (15.27). The total energy per site for any J is thus given by

$$\frac{E}{N} = J \frac{1}{N} \sum_{n=1}^{\infty} \sum_{\alpha=1}^{M_n} \frac{n}{(\lambda_{\alpha}^n)^2 + (n^2/4)} - h\left(1 - \frac{2}{N} \sum_{n=1}^{\infty} nM_n\right)$$
$$= -h + \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} d\lambda \ (2\pi J a_n(\lambda) + 2nh) \rho_n(\lambda).$$
(16.32)

The total entropy per site is

$$\frac{S}{N} = \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}\lambda \,\left\{ (\rho_n + \tilde{\rho}_n) \ln(\rho_n + \tilde{\rho}_n) - \rho_n \ln\rho_n - \tilde{\rho}_n \ln\tilde{\rho}_n \right\}.$$
(16.33)

The equilibrium state of the isotropic Heisenberg chain at temperature T is described by the equilibrium particle densities $\{\rho^{eq}\}$ and hole densities $\{\tilde{\rho}^{eq}\}$. Introducing the free energy

$$F = E - TS, \tag{16.34}$$

the densities are determined by the variational condition

$$\delta F\Big|_{\rho=\rho^{eq},\tilde{\rho}=\tilde{\rho}^{eq}} = 0, \qquad \delta F = \delta E - T\delta S.$$
(16.35)

The functional variations of the energy and of the entropy with respect to $\{\rho_n\}$ and $\{\tilde{\rho}_n\}$ are given by

$$\frac{1}{N}\delta E = \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} d\lambda \left\{ 2\pi J a_n(\lambda) + 2nh \right\} \delta\rho_n(\lambda), \tag{16.36}$$

$$\frac{1}{N}\delta S = \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}\lambda \,\left\{ \ln\left(1 + \frac{\tilde{\rho}_n}{\rho_n}\right)\delta\rho_n + \ln\left(1 + \frac{\rho_n}{\tilde{\rho}_n}\right)\delta\tilde{\rho}_n \right\}.$$
(16.37)

The constraint (16.25) implies

$$\delta\tilde{\rho}_n = -\sum_{m=1}^{\infty} A_{nm} * \delta\rho_m.$$
(16.38)

Using the symmetricity of the A-matrix, the condition (16.35) yields

$$\ln(1+\eta_n) = \frac{1}{T} \left(2\pi J a_n + 2nh \right) + \sum_{m=1}^{\infty} A_{nm} * \ln\left(1+\eta_m^{-1}\right), \qquad n = 1, 2, \dots, (16.39)$$

where $\eta_n(\lambda) = \tilde{\rho}_n^{eq}(\lambda)/\rho_n^{eq}(\lambda)$. Forming the convolution of this equation with the inverse function A^{-1} , noting that $\hat{a}_n(\omega) = \hat{s}(\omega)\hat{A}_{n,1}(\omega)$ and using the relations

$$\sum_{n=1}^{\infty} (A_{n'n}^{-1} * a_n)(\lambda) = s(\lambda)\delta_{n'1}, \qquad \sum_{n=1}^{\infty} A_{n'n}^{-1} * n = 0,$$
(16.40)

we finally arrive at an infinite sequence of TBA equations

$$\ln \eta_1(\lambda) = \frac{2\pi J}{T} s(\lambda) + \int_{-\infty}^{\infty} \mathrm{d}\lambda' \, s(\lambda - \lambda') \ln \left[1 + \eta_2(\lambda')\right], \tag{16.41}$$

$$\ln \eta_n(\lambda) = \int_{-\infty}^{\infty} d\lambda' \, s(\lambda - \lambda') \ln \left\{ \left[1 + \eta_{n-1}(\lambda') \right] \left[1 + \eta_{n+1}(\lambda') \right] \right\}, \qquad n \ge 2.$$
(16.42)

These equations are not complete since they do not contain the field h. Let us consider the leading $n \to \infty$ asymptotic of the generic Eq. (16.39). Since $\lim_{n\to\infty} a_n(\lambda) \to 0$, the leading asymptotic is

$$\lim_{n \to \infty} \frac{\ln \eta_n(\lambda)}{n} = \frac{2h}{T}.$$
(16.43)

Note that the TBA functions possess the symmetry $\eta_n(\lambda) = \eta_n(-\lambda)$.

In order to express the free energy per site f = F/N in terms of the TBA functions $\{\eta_n(\lambda)\}$, we use Eqs. (16.32)–(16.34) to write

$$f = -h + \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} d\lambda \left\{ \left[2\pi J a_n(\lambda) + 2nh \right] \rho_n(\lambda) - T \rho_n(\lambda) \ln[1 + \eta_n(\lambda)] - T \tilde{\rho}_n(\lambda) \ln[1 + \eta_n^{-1}(\lambda)] \right\}.$$
(16.44)

Eliminating $\tilde{\rho}_n$ via the relation (16.25), the coefficient of ρ_n vanishes by virtue of the TBA equations (16.39) and we obtain

$$f = -h - T \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} d\lambda \ a_n(\lambda) \ln\left[1 + \eta_n^{-1}(\lambda)\right].$$
(16.45)

This formula can be further simplified. The n = 1 case of Eq. (16.39) reads

$$\ln(1+\eta_1) = \frac{1}{T}(2\pi J a_1 + 2h) + \sum_{m=1}^{\infty} (a_{m-1} + a_{m+1}) * \ln\left(1+\eta_m^{-1}\right).$$
(16.46)

Applying on this equation the operator $\int_{-\infty}^{\infty} d\lambda \, s(\lambda)$ and using the relation

$$\hat{s}(\omega) \left[\hat{a}_{n-1}(\omega) + \hat{a}_{n+1}(\omega) \right] = \hat{a}_n(\omega),$$
(16.47)

we have

$$\int_{-\infty}^{\infty} d\lambda \, s(\lambda) \ln[1+\eta_1(\lambda)] = \frac{2\pi J}{T} \int_{-\infty}^{\infty} d\lambda \, s(\lambda) a_1(\lambda) + \frac{h}{T} + \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} d\lambda \, a_n(\lambda) \ln\left[1+\eta_n^{-1}(\lambda)\right].$$
(16.48)

The expression (16.45) is thus equivalent to the formula

$$f = 2J\ln 2 - T \int_{-\infty}^{\infty} \mathrm{d}\lambda \, s(\lambda) \ln\left[1 + \eta_1(\lambda)\right], \tag{16.49}$$

which contains only the lowest TBA function.

At a given nonzero (finite) temperature, the TBA equations can be solved only numerically; for a review, see the monography [30]. However, they can also serve as a systematic tool for developing the high-temperature and low-temperature expansions of the free energy.

16.2 High-temperature expansion

For the isotropic XXX Heisenberg chain, the high-temperature expansion of the free energy per site can be performed directly from the definition

$$\frac{f}{T} = -\frac{1}{N}\ln\operatorname{Tr}\exp(-H/T).$$
(16.50)

The isotropic Hamiltonian (16.1) can be decomposed as follows $H = H_0 + JH_1$, where the operators

$$H_0 = -h \sum_{n=1}^{N} \boldsymbol{\sigma}_n^z, \qquad H_1 = -\frac{1}{2} \sum_{n=1}^{N} \left(\vec{\boldsymbol{\sigma}}_n \cdot \vec{\boldsymbol{\sigma}}_{n+1} - 1 \right)$$
(16.51)

commute with one another, $[H_0, H_1] = 0$. Thus the exponential of H can be expanded as a power series in J/T,

$$\exp(-H/T) = \exp(-H_0/T) \left[1 - \frac{J}{T} \frac{H_1}{1!} + \left(\frac{J}{T}\right)^2 \frac{H_1^2}{2!} - \cdots \right].$$
 (16.52)

This implies the standard cumulant expansion for the free energy

$$\frac{f}{T} = -\frac{1}{N}\ln\operatorname{Tr}\exp(-H_0/T) + \frac{J}{T}\frac{\langle H_1 \rangle}{1!N} - \left(\frac{J}{T}\right)^2\frac{\langle H_1^2 \rangle - \langle H_1 \rangle^2}{2!N} + \cdots,$$
(16.53)

where the symbol

$$\langle \cdots \rangle \equiv \frac{\text{Tr} \cdots \exp(-H_0/T)}{\text{Tr} \exp(-H_0/T)}$$
(16.54)

denotes the equilibrium average with the Hamiltonian H_0 . The evaluation of the mean values $\langle H_1 \rangle$, $\langle H_1^2 \rangle$, etc. is easy. In this way, we obtain the systematic J/T expansion of the free energy at fixed h/T,

$$\frac{f}{T} = -\ln\left[2\cosh(h/T)\right] + \frac{J}{T}\frac{1}{2\cosh^2(h/T)} - \frac{J^2}{8T^2}\left[3 + 2\tanh^2(h/T) - 3\tanh^4(h/T)\right] + O\left[\left(\frac{J}{T}\right)^3\right].$$
(16.55)

In what follows, we rederive this expansion by using the TBA equations (16.41)–(16.43), complemented by the formula (16.49) for the free energy.

In lowest expansion order $J/T \to 0$, the functions $\eta_n(\lambda)$ are independent of λ . Since $\int_{-\infty}^{\infty} d\lambda \ s(\lambda) = 1/2$, the TBA equations become

$$\eta_n^2 = (1 + \eta_{n-1}) (1 + \eta_{n+1}), \qquad n \ge 2; \tag{16.56}$$

$$\eta_1^2 = 1 + \eta_2, \qquad \lim_{n \to \infty} \frac{\ln \eta_n}{n} = \frac{2h}{T}.$$
 (16.57)

The general solution of the second-order difference equation (16.56) is

$$\eta_n = \left[\frac{az^n - (az^n)^{-1}}{z - z^{-1}}\right]^2 - 1.$$
(16.58)

The parameters a and z are determined by the "boundary" conditions (16.57) as follows: a = z, $z = \exp(h/T)$. Hence

$$\eta_n = \left[\frac{\sinh[(n+1)h/T]}{\sinh(h/T)}\right]^2 - 1.$$
(16.59)

The substitution of $\eta_1 = [2\cosh(h/T)]^2 - 1$ into the representation (16.49) reproduces correctly the leading term of the expansion (16.55).

At higher expansion orders in J/T, we formally write $\ln[1 + \eta_n(\lambda)]$ as the expansion

$$\ln\left[1+\eta_n(\lambda)\right] = \ln\left(\frac{\alpha_n}{\alpha_n-1}\right) + \sum_{m=1}^{\infty} \left(\frac{J}{T}\right)^m f_n^{(m)}(\lambda),$$
(16.60)

$$\alpha_n = \frac{\sinh^2 \left[(n+1)h/T \right]}{\sinh(nh/T)\sinh\left[(n+2)h/T \right]}.$$
(16.61)

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The corresponding expansion of $\ln \eta_n(\lambda)$, to first order in J/T, takes the form

$$\ln \eta_n(\lambda) = \ln \left(\frac{1}{\alpha_n - 1}\right) + \frac{J}{T} \alpha_n f_n^{(1)}(\lambda) + O\left[\left(\frac{J}{T}\right)^2\right].$$
(16.62)

Substituting the above expansions into the TBA equations and considering only terms of order J/T results in a chain of coupled linear integral equations

$$\alpha_n f_n^{(1)} = s * \left[f_{n-1}^{(1)} + f_{n+1}^{(1)} \right], \qquad n \ge 2;$$
(16.63)

$$\alpha_1 f_1^{(1)} = 2\pi s + s * f_2^{(1)}, \qquad \lim_{n \to \infty} \frac{\alpha_n f_n^{(1)}}{n} = 0.$$
(16.64)

The Fourier transform of Eq. (16.63) takes the form

$$\left(e^{\omega/2} + e^{-\omega/2}\right)\alpha_n \hat{f}_n^{(1)}(\omega) = \hat{f}_{n-1}^{(1)}(\omega) + \hat{f}_{n+1}^{(1)}(\omega).$$
(16.65)

The solution of this difference equation, respecting the boundary conditions (16.64), is

$$\hat{f}_{n}^{(1)}(\omega) = \frac{\pi}{\cosh(h/T)} \left\{ \frac{\sinh[(n+2)h/T]}{\sinh[(n+1)h/T]} e^{-n|\omega|/2} - \frac{\sinh(nh/T)}{\sinh[(n+1)h/T]} e^{-(n+2)|\omega|/2} \right\}.$$
(16.66)

The inverse Fourier transform of this formula, taken at n = 1, gives

$$f_1^{(1)}(\lambda) = \frac{\pi}{\cosh(h/T)} \left\{ \frac{\sinh(3h/T)}{\sinh(2h/T)} a_1(\lambda) - \frac{\sinh(h/T)}{\sinh(2h/T)} a_3(\lambda) \right\}.$$
 (16.67)

 $f_1^{(1)}(\lambda)$ is the coefficient of the term of order J/T in the expansion (16.60). The substitution of this term into (16.49) reproduces correctly the second term of the high-temperature expansion (16.55).

Higher-order terms in J/T can be calculated analogously by solving the corresponding sets of linear integral equations for $f_n^{(2)}(\lambda)$, $f_n^{(3)}(\lambda)$, etc., with inhomogeneous terms induced by lower-order coefficients $f_n^{(l)}$.

16.3 Low-temperature expansion

Since in the limit $T \to 0$ the functions $\ln \eta_n$ diverge as 1/T, we introduce the "energy functions"

$$\epsilon_n(\lambda) = T \ln \eta_n(\lambda), \qquad \epsilon(\lambda) = \epsilon(-\lambda).$$
 (16.68)

The TBA sequence of integral equations for $\{\epsilon_n\}$ reads

$$\epsilon_1 = 2\pi J s + T s * \ln\left(1 + e^{\epsilon_2/T}\right), \qquad (16.69)$$

$$\epsilon_n = T s * \ln\left[\left(1 + e^{\epsilon_{n-1}/T}\right)\left(1 + e^{\epsilon_{n+1}/T}\right)\right], \qquad n \ge 2$$
(16.70)

and the asymptotic condition is

$$\lim_{n \to \infty} \frac{\epsilon_n}{n} = 2h. \tag{16.71}$$

The free energy per site is expressible in two ways

$$f(T,h) = -h - T \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} d\lambda \, a_n(\lambda) \ln\left(1 + e^{-\epsilon_n(\lambda)/T}\right)$$
$$= 2J \ln 2 - T \int_{-\infty}^{\infty} d\lambda \, s(\lambda) \ln\left(1 + e^{\epsilon_1(\lambda)/T}\right).$$
(16.72)

16.3.1 Ferromagnet

For J = +1, it follows from the form of the TBA equations that

$$\epsilon_n(\lambda) \ge 0 \qquad \text{for all } n \ge 1.$$
 (16.73)

Due to this positivity property, the logarithmic terms in the TBA equations can be expanded for small T as follows

$$T\ln\left(1+\mathrm{e}^{\epsilon/T}\right) = \epsilon + T\mathrm{e}^{-\epsilon/T} + \cdots \qquad \text{for } \epsilon \ge 0.$$
 (16.74)

• T = 0: In leading $T \to 0$ order, $\epsilon_n = \epsilon_n^{(0)}$, the TBA equations become

$$\epsilon_1^{(0)} = 2\pi s + s * \epsilon_2^{(0)}, \tag{16.75}$$

$$\epsilon_n^{(0)} = s * \left(\epsilon_{n-1}^{(0)} + \epsilon_{n+1}^{(0)} \right) \qquad n \ge 2,$$
(16.76)

with $\lim_{n\to\infty} \epsilon_n^{(0)}(\lambda)/n = 2h$. This set of equations is solvable by using the Fourier-transform method. The final result is

$$\epsilon_n^{(0)}(\lambda) = 2\pi a_n(\lambda) + 2nh, \qquad n = 1, 2, \dots$$
 (16.77)

The free energy at zero temperature is found to be

$$f(0,h) = 2\ln 2 - \int_{-\infty}^{\infty} d\lambda \ s(\lambda)\epsilon_1^{(0)}(\lambda) = -h.$$
 (16.78)

This is nothing but the energy of the ferromagnetic ground-state with all spins up.

• Small T: In next order, we substitute $\epsilon_n = \epsilon_n^{(0)} + \epsilon_n^{(1)}$ into the TBA equations and expand the logarithms up to the order indicated in (16.74). The contribution of the exponentials $e^{-\epsilon_n^{(0)}/T}$ with $n \ge 2$ is negligible in comparison with the one of $e^{-\epsilon_1^{(0)}/T}$ as $T \to 0$. Taking into account the leading TBA equations (16.75) and (16.76), we get

$$\epsilon_1^{(1)} = s * \epsilon_2^{(1)} \tag{16.79}$$

$$\epsilon_2^{(1)} = s * \left(\epsilon_1^{(1)} + \epsilon_3^{(1)}\right) + T s * e^{-\epsilon_1^{(0)}/T}$$
(16.80)

$$\epsilon_n^{(1)} = s * \left(\epsilon_{n-1}^{(1)} + \epsilon_{n+1}^{(1)} \right) \quad \text{for } n \ge 3.$$
(16.81)

The asymptotic condition is $\lim_{n\to\infty} \epsilon_n^{(1)}/n = 0$. The Fourier-transform method yields

$$\begin{aligned}
\epsilon_n^{(1)} &= T(a_{n-1} + a_{n+1}) * e^{-\epsilon_1^{(0)}/T} & \text{for } n \ge 2, \\
\epsilon_1^{(1)} &= T a_2 * e^{-\epsilon_1^{(0)}/T}.
\end{aligned}$$
(16.82)
(16.83)

¹⁾ =
$$T a_2 * e^{-\epsilon_1^{(0)}/T}$$
. (16.83)

The difference of the free energies at small T and at T = 0 is given by

$$f(T,h) - f(0,h) = -\int_{-\infty}^{\infty} d\lambda \, s(\lambda) \left[\epsilon_1^{(1)}(\lambda) + T e^{-\epsilon_1^{(0)}/T} \right].$$
(16.84)

Inserting here $\epsilon_1^{(1)}$ and using the equality $\hat{s}(\omega)\hat{a}_2(\omega) = \hat{a}_1(\omega) - \hat{s}(\omega)$, we obtain

$$f(T,h) - f(0,h) = -T e^{-2h/T} \int_{-\infty}^{\infty} d\lambda \, a_1(\lambda) e^{-2\pi a_1(\lambda)/T}.$$
(16.85)

The substitution $\lambda = \lambda'/\sqrt{T}$ permits us to evaluate the $T \to 0$ limit of the integral, with the result

$$f(T,h) - f(0,h) = -\frac{T^{3/2}}{2\sqrt{\pi}} e^{-2h/T}.$$
(16.86)

16.3.2 Antiferromagnet

For J = -1, from the form of the TBA equations we conclude that

$$\epsilon_n(\lambda) \ge 0 \qquad \text{for } n \ge 2.$$
 (16.87)

The small-T expansion (16.74) is applied for these functions. The $\epsilon_1(\lambda)$ can have either sign. Let us introduce the notation

$$\epsilon_1^+ \equiv \frac{1}{2} (\epsilon_1 + |\epsilon_1|), \qquad \epsilon_1^- \equiv \frac{1}{2} (\epsilon_1 - |\epsilon_1|).$$
 (16.88)

In the small-T limit, we have

$$\lim_{T \to 0} T \ln \left(1 + e^{\pm \epsilon_1/T} \right) = \pm \epsilon_1^{\pm}.$$
(16.89)

• T = 0: In leading $T \to 0$ order, $\epsilon_n = \epsilon_n^{(0)}$, the TBA equations read

$$\epsilon_1^{(0)} = -2\pi s + s \ast \epsilon_2^{(0)}, \tag{16.90}$$

$$\epsilon_2^{(0)} = s * \epsilon_1^{(0)+} + s * \epsilon_3^{(0)}, \tag{16.91}$$

$$\epsilon_n^{(0)} = s * \left(\epsilon_{n-1}^{(0)} + \epsilon_{n+1}^{(0)}\right) \qquad n \ge 3.$$
(16.92)

The solution can be deduced with the aid of Fourier transforms:

$$\epsilon_n^{(0)} = a_{n-1} * \epsilon_1^{(0)+} + 2(n-1)h \qquad n \ge 2.$$
(16.93)

The equation which determines $\epsilon_1^{(0)}$ is

$$\epsilon_1^{(0)} = -2\pi s + h + (s * a_1) * \epsilon_1^{(0)+}.$$
(16.94)

An alternative equation can be derived by substituting here $\epsilon_1^{(0)+} = \epsilon_1^{(0)} - \epsilon_1^{(0)-}$ and then Fourier solving for $\epsilon_1^{(0)}$ in terms of $\epsilon_1^{(0)-}$,

$$\epsilon_1^{(0)} = -2\pi a_1 + 2h - a_2 * \epsilon_1^{(0)-}.$$
(16.95)

For h = 0, since $s(\lambda)$ is positive for all λ , we have $\epsilon_1^{(0)+} = 0$ and Eq. (16.94) has the solution

$$\epsilon_1^{(0)}(\lambda) = -2\pi s(\lambda) = -\frac{\pi}{\cosh(\pi\lambda)}.$$
(16.96)

This is just the excitation energy function $\epsilon(\lambda)$ for the isotropic antiferromagnet, i.e. minus $\Delta E(\lambda)$ given by (15.83). The free energy can be calculated in two ways, see Eq. (16.72). Firstly,

$$f(0,0) = -h - T \int_{-\infty}^{\infty} d\lambda \, a_1(\lambda) \ln\left(1 + e^{-\epsilon_1(\lambda)/T}\right)$$
$$= \int_{-\infty}^{\infty} d\lambda \, a_1(\lambda) \epsilon_1^{(0)-}(\lambda) = -2\ln 2.$$
(16.97)

This is the ground-state energy of the isotropic antiferromagnet in zero field. Secondly,

$$f(0,0) = -2\ln 2 - \int_{-\infty}^{\infty} d\lambda \, s(\lambda) \epsilon_1^{(0)+}(\lambda) = -2\ln 2.$$
(16.98)

When h > 0 and simultaneously $2h - 2\pi a_1(0) < 0$, i.e. h < 2, $\epsilon_1^{(0)}(\lambda)$ is a monotonically increasing function for $\lambda \ge 0$. As follows from Eq. (16.95), it is negative for $\lambda = 0$ and, because $a_1(\infty)$ and $a_2(\infty)$ are zero, goes to 2h for $\lambda \to \infty$. Thus $\epsilon_1^{(0)}(\lambda)$ has just two zeros at $\pm b$ (b > 0). Eq. (16.95) can be rewritten as

$$\epsilon_1^{(0)}(\lambda) = -2\pi a_1(\lambda) + 2h - \int_{-b}^{b} d\lambda' \, a_2(\lambda - \lambda')\epsilon_1^{(0)}(\lambda').$$
(16.99)

Since a_1 and a_2 , given by (16.26), are simultaneously expressible as

$$a_1(\lambda) = \frac{k'(\lambda)}{2\pi}$$
 and $a_2(\lambda) = \frac{\theta'(\lambda)}{2\pi}$, (16.100)

this equation is identical to the previous one (15.68) for the zero-temperature $\epsilon(\lambda)$.

• Small *T*: As before, the contribution of the exponentials $e^{-\epsilon_n^{(0)}/T}$ with $n \ge 2$ is negligible in next order. Comparing the original n = 2 equation (16.70) with the linearized one (16.91) it is clear that we should substitute $\epsilon_1^{(0)+} \to T \ln(1 + e^{-\epsilon_1/T})$ in Eq. (16.94), to obtain

$$\epsilon_1 = -2\pi s + h + T(s * a_1) * \ln(1 + e^{\epsilon_1/T}).$$
(16.101)

This equation can be straightforwardly transformed to

$$\epsilon_1 = -2\pi a_1 + 2h + T a_2 * \ln(1 + e^{-\epsilon_1/T}).$$
(16.102)

If $T \ll 4-2h$, $\epsilon_1(\lambda)$ has two zeros at $\pm b_T$ ($b_0 = b$) also for finite T; $\epsilon_1(\lambda) < 0$ for $|\lambda| < b_T$ and $\epsilon_1(\lambda) > 0$ for $|\lambda| > b_T$. We write $\epsilon_1 = \epsilon_1^{(0)} + \epsilon_1^{(1)}$ in (16.102) and subtract the linearized equation (16.99). The result is

$$\epsilon_1^{(1)}(\lambda) + \int_{-b}^{b} \mathrm{d}\lambda' \, a_2(\lambda - \lambda')\epsilon_1^{(1)}(\lambda') = \left[\int_{b_T}^{b} + \int_{-b}^{-b_T}\right] \mathrm{d}\lambda' \, a_2(\lambda - \lambda')\epsilon_1(\lambda') + I(\lambda), \tag{16.103}$$

where the inhomogeneous term $I(\lambda)$ is given by

$$I = T a_2 * \ln \left(1 + e^{-|\epsilon_1|/T} \right).$$
(16.104)

For $T \to 0$, the dominant contribution to this integral comes from the neighborhood of the zeros of ϵ_1 . Expanding $\epsilon_1(\lambda)$ around b_T ,

$$\epsilon_1(\lambda) = \epsilon'_1(b_T)(\lambda - b_T) + O\left((\lambda - b_T)^2\right),\tag{16.105}$$

and analogously around $-b_T$, the leading T-dependence of the inhomogeneous term $I(\lambda)$ becomes

$$I(\lambda) = \frac{T^2}{\epsilon'_1(b_T)} \left[a_2(\lambda - b_T) + a_2(\lambda + b_T) \right] \int_{-\infty}^{\infty} du \ln \left(1 + e^{-|u|} \right)$$

= $\frac{\pi^2 T^2}{6\epsilon'_1(b_T)} \left[a_2(\lambda - b_T) + a_2(\lambda + b_T) \right].$ (16.106)

Since $\epsilon_1(\pm b_T) = 0$, the first two terms on the rhs of Eq. (16.103) are of order $(b - b_T)^2$. The lhs of the same equation is expected to be of order $b - b_T$, so $b - b_T = O(T^2)$. Neglecting terms of order $O(T^3)$, Eq. (16.103) can be rewritten as

$$\epsilon_1^{(1)}(\lambda) + \int_{-b}^{b} \mathrm{d}\lambda' \, a_2(\lambda - \lambda') \epsilon_1^{(1)}(\lambda') = \frac{\pi^2 T^2}{6\epsilon_1^{(0)'}(b)} \left[a_2(\lambda - b_T) + a_2(\lambda + b_T) \right]. \quad (16.107)$$

With regard to the definition (16.100) of $a_2(\lambda)$, we conclude that

$$\epsilon_1^{(1)}(\lambda) = \frac{\pi^2 T^2}{3\epsilon_1^{(0)'}(b)} C(\lambda), \tag{16.108}$$

where $C(\lambda) = C_{+}(\lambda) + C_{-}(\lambda)$ with $C_{\pm}(\lambda)$ obeying the integral equations (14.43).

We need the explicit expression for $\epsilon_1^{(0)'}(b)$. Differentiating first (16.99) with respect to λ and then applying an integration by parts, we have

$$\epsilon_1^{(0)'}(\lambda) = 2\pi V(\lambda), \tag{16.109}$$

where $V(\lambda)$ satisfies the integral equation

$$V(\lambda) + \int_{-b}^{b} \mathrm{d}\lambda' \, a_2(\lambda - \lambda')V(\lambda') = -\frac{\mathrm{d}}{\mathrm{d}\lambda}a_1(\lambda).$$
(16.110)

To evaluate the free energy per site, we prefer to use the formula (16.97) which gives

$$f(T,h) - f(0,h) = -T \int_{-\infty}^{\infty} d\lambda \, a_1(\lambda) \ln\left(1 + e^{-|\epsilon_1(\lambda)|/T}\right) + \int_{-b_T}^{b_T} d\lambda \, a_1(\lambda) \epsilon_1(\lambda) - \int_{-b}^{b} d\lambda \, a_1(\lambda) \epsilon_1^{(0)}(\lambda) = -\frac{\pi^2 T^2}{3\epsilon_1^{(0)'}(b)} \left[a_1(b) - \int_{-b}^{b} d\lambda \, a_1(\lambda) C(\lambda)\right].$$
(16.111)

Taking advantage of the symmetries $a_1(\lambda) = a_1(-\lambda)$ and $C_{\pm}(\lambda) = C_{\mp}(-\lambda)$, in terms of $D(\lambda) = 2C_{-}(\lambda)$ we have $\int_{-b}^{b} d\lambda a_1(\lambda)C(\lambda) = \int_{-b}^{b} d\lambda a_1(\lambda)D(\lambda)$. Setting in Eq. (14.47) $e(\lambda) = -k'(\lambda) = -2\pi a_1(\lambda)$, the bracket on the rhs of (16.111) is equal to $\rho(b)$, where the density of λ 's is defined in (13.96), i.e.

$$\rho(\lambda) + \int_{-b}^{b} \mathrm{d}\lambda' \, a_2(\lambda - \lambda')\rho(\lambda') = a_1(\lambda). \tag{16.112}$$

We conclude that

$$f(T,h) = f(0,h) - \frac{\pi T^2}{6} \frac{\rho(b)}{V(b)} + O(T^3).$$
(16.113)

The ratio $\rho(b)/V(b)$ can be easily evaluated in the limit $h \to 0 \ (b \to \infty)$ with the aid of the Wiener-Hopf technique, see Sect. 14. In particular, we find

$$\rho(b) \sim \zeta \lim_{x \to 0^+} T(x), \qquad V(b) \sim \pi \zeta \lim_{x \to 0^+} T(x),$$
(16.114)

which implies that $\rho(b)/V(b) = 1/\pi$ in the limit $b \to \infty$. The free energy per site is given by

$$f(T,0) = -2\ln 2 - \frac{T^2}{6} + o(T^2).$$
(16.115)

To lowest order in temperature, the specific heat at h = 0 is given by

$$C = -T\frac{\partial^2}{\partial T^2}f(T, h = 0) = \frac{1}{3}T.$$
(16.116)

According to the conformal invariance theory [31, 32], the free energy per site of a critical quantum chain exhibits the small-T expansion

$$f = e_0 - \frac{\pi c}{6v_s} T^2 + \cdots,$$
(16.117)

where v_s is the sound velocity and c is the central charge. For the isotropic antiferromagnet, we have $v_s = \pi$ and therefore c = 1.

17 XXZ Heisenberg chain: Thermodynamics without strings

The above derivation of the thermodynamics of the isotropic Heisenberg chain was based on the string hypothesis which was criticized many times. The result is an infinite sequence of coupled TBA integral equations. From among alternative approaches which avoid the manipulations with strings, we present the "quantum transfer matrix" (QTM) method [33–39], It is based on a lattice path-integral representation of the partition function for the one-dimensional Heisenberg model and leads to a finite set of non-linear integral equations.

17.1 Quantum transfer matrix

We studied in Sect. 8.3 the classical two-dimensional six-vertex model with vertex weights $a(\lambda)$, $b(\lambda)$ and $c(\lambda)$. The corresponding S-matrix $S_{12}(\lambda_1, \lambda_2) \equiv S_{12}(\lambda_1 - \lambda_2)$ is defined by

$$S_{12} = \frac{a+b}{2} + \frac{c}{2} \left(\boldsymbol{\sigma}_1^x \boldsymbol{\sigma}_2^x + \boldsymbol{\sigma}_1^y \boldsymbol{\sigma}_2^y \right) + \frac{a-b}{2} \boldsymbol{\sigma}_1^z \boldsymbol{\sigma}_2^z.$$
(17.1)

Within the trigonometric parametrization of vertex weights (8.27), the S-matrix satisfies the YBE

$$S_{12}(\lambda_1, \lambda_2)S_{13}(\lambda_1, \lambda_3)S_{23}(\lambda_2, \lambda_3) = S_{23}(\lambda_2, \lambda_3)S_{13}(\lambda_1, \lambda_3)S_{12}(\lambda_1, \lambda_2).$$
(17.2)

In the paramagnetic region, we shall use the standard notation $\eta \equiv \gamma$. Rescaling λ by $\gamma/2$ and dividing all vertex weights by $\sin(\gamma + \gamma \lambda/2)$, we have

$$a(\lambda) = 1,$$
 $b(\lambda) = \frac{\sin(\gamma\lambda/2)}{\sin(\gamma+\gamma\lambda/2)},$ $c(\lambda) = \frac{\sin\gamma}{\sin(\gamma+\gamma\lambda/2)}.$ (17.3)

With these vertex weights, the S-matrix satisfies the initial condition $S(\lambda = 0) = \mathcal{P}$, where \mathcal{P} is the permutation operator. In algebraic manipulations which follows, we shall need anticlockwise and clockwise 90° rotations of the S-matrix in the edge-state configuration space around the vertex:

$$\bar{S}^{\sigma_1 \sigma_2}_{\sigma_1' \sigma_2'}(\lambda_1, \lambda_2) = S^{\sigma_2 \sigma_1'}_{\sigma_2' \sigma_1}(\lambda_2, \lambda_1), \qquad \tilde{S}^{\sigma_1 \sigma_2}_{\sigma_1' \sigma_2'}(\lambda_1, \lambda_2) = S^{\sigma_2' \sigma_1}_{\sigma_2 \sigma_1'}(\lambda_2, \lambda_1).$$
(17.4)

For a row of L sites, the row-to-row transfer matrix reads

$$T(\lambda)^{\sigma_1\dots\sigma_L}_{\sigma'_1\dots\sigma'_L} = \sum_{\{\gamma\}} \prod_{l=1}^L S^{\sigma_l\gamma_l}_{\sigma'_l\gamma_{l+1}}(\lambda).$$
(17.5)

 $T(\lambda = 0)$ reduces to the right-shift operator T_R . The Hamiltonian of the XXZ Heisenberg chain with the anisotropy parameter $|\Delta| < 1$,

$$H = \frac{1}{2} \sum_{l=1}^{L} \left[\left(\boldsymbol{\sigma}_{l}^{x} \boldsymbol{\sigma}_{l+1}^{x} + \boldsymbol{\sigma}_{l}^{y} \boldsymbol{\sigma}_{l+1}^{y} \right) + \cos \gamma \left(\boldsymbol{\sigma}_{l}^{z} \boldsymbol{\sigma}_{l+1}^{z} - 1 \right) \right]$$

$$\equiv -\frac{1}{2} \sum_{l=1}^{L} \left[\left(\boldsymbol{\sigma}_{l}^{x} \boldsymbol{\sigma}_{l+1}^{x} + \boldsymbol{\sigma}_{l}^{y} \boldsymbol{\sigma}_{l+1}^{y} \right) - \cos \gamma \left(\boldsymbol{\sigma}_{l}^{z} \boldsymbol{\sigma}_{l+1}^{z} - 1 \right) \right], \qquad (17.6)$$

is obtained as the logarithmic derivative of the transfer matrix at $\lambda = 0$,

$$H = 2 \frac{\sin \gamma}{\gamma} \frac{\mathrm{d}}{\mathrm{d}\lambda} \ln T(\lambda) \Big|_{\lambda=0}.$$
(17.7)

Thus,

$$T(\lambda) = T_R \left[1 + \frac{\gamma}{2\sin\gamma} \lambda H + O(\lambda^2) \right].$$
(17.8)

The "adjoint" transfer matrix $\overline{T}(\lambda)$, defined as a product of $\overline{S}(-\lambda)$ in analogy with (17.5), has the small- λ expansion

$$\bar{T}(\lambda) = T_L \left[1 + \frac{\gamma}{2\sin\gamma} \lambda H + O(\lambda^2) \right],$$
(17.9)

where $T_L = T_R^{-1}$ is the left-shift operator.

Due to the periodic boundary conditions, the right- and left-shift operators commute with the Hamiltonian, $[T_R, H] = [T_L, H] = 0$. The Trotter identity allows us to express the Boltzmann factor in the following way

$$e^{-\beta H} = \lim_{N \to \infty} \left[T(-\tau) \bar{T}(-\tau) \right]^{N/2}, \qquad \tau = 2 \frac{\sin \gamma}{\gamma} \frac{\beta}{N}, \tag{17.10}$$

where the large number N is even. The partition function Z_L of the XXZ Heisenberg chain of L sites is thus expressible as follows

$$Z_{L} = \lim_{N \to \infty} Z_{L,N}, \qquad Z_{L,N} = \text{Tr} \left[T(-\tau) \bar{T}(-\tau) \right]^{N/2}.$$
(17.11)

 $Z_{L,N}$ can be interpreted as the partition function of a staggered vertex model with N/2 + N/2 alternating rows corresponding to the transfer matrices $T(-\tau)$ and $\overline{T}(-\tau)$. We are allowed to change the transfer direction from rows to columns. The column-to-column "quantum transfer matrix" T^{QTM} is the $\lambda = 0$ member of the family of matrices:

$$T^{\text{QTM}}(\lambda)^{\sigma_1...\sigma_N}_{\sigma'_1...\sigma'_N} = \sum_{\{\gamma\}} \prod_{n=1}^{N/2} S^{\sigma_{2n-1}\gamma_{2n-1}}_{\sigma'_{2n-1}\gamma_{2n}}(\lambda-\tau) \tilde{S}^{\sigma_{2n}\gamma_{2n}}_{\sigma'_{2n}\gamma_{2n+1}}(\lambda+\tau).$$
(17.12)

Since $Z_{L,N} = \text{Tr}(T^{\text{QTM}})^L$, the free energy per site f of the infinite quantum spin chain is given by

$$-\beta f = \lim_{L \to \infty} \frac{1}{L} \ln Z_L = \lim_{N \to \infty} \ln t_{\max}(0), \qquad (17.13)$$

where $t_{\max}(0)$ is the largest eigenvalue of $T^{\text{QTM}}(0)$. In formulating this result, we interchanged the limits $L \to \infty$ and $N \to \infty$ which is possible due to the theorems presented in [40, 41]. All other eigenvalues of $T^{\text{QTM}}(0)$ are separated from $t_{\max}(0)$ by a finite gap, even in the limit $N \to \infty$. Note that $t_{\max}(0)$ depends on the parameter $\tau \propto 1/N$, so the treatment of the $N \to \infty$ limit is a delicate issue. In the presence of an external magnetic field h coupled to $2S^z = \sum_l \sigma_l^z$, the corresponding two-dimensional vertex model is modified by a horizontal seam along which each link variable $\sigma = \pm$ carries the Boltzmann weight $e^{\pm\beta h}$. Passing to the column transfer direction, the link variable is identified with the auxiliary ξ -space of the monodromy matrix (7.44). In the representation of the monodromy matrix (8.31), the presence of the magnetic field is reflected through the additional Boltzmann factors in $e^{\beta h}A(\lambda)$ and $e^{-\beta h}D(\lambda)$. An alternative approach [34,35] is to consider the twisted relation between spin operators after a translation by N sites:

$$\boldsymbol{\sigma}_{n+N}^{x} \pm \mathrm{i}\boldsymbol{\sigma}_{n+N}^{y} = \mathrm{e}^{\pm\beta h} \left[\boldsymbol{\sigma}_{n}^{x} \pm \mathrm{i}\boldsymbol{\sigma}_{n}^{y} \right], \qquad \boldsymbol{\sigma}_{n+N}^{z} = \boldsymbol{\sigma}_{n}^{z}.$$
(17.14)

17.2 Bethe ansatz equations

We want to diagonalize the quantum transfer matrix (17.12). It is composed of alternating S and \tilde{S} matrices, with differently shifted spectral parameter λ . The introduction of the spectral parameter λ in (17.12), although physically interesting is only the $\lambda = 0$ case, is related to the existence of a commuting family of the quantum transfer matrices generated by this λ . The commutation property will be proven in what follows by using the QISM explained in Sect. 7.3.

It is easy to derive the analogy of the YBE (17.2) involving the \hat{S} -matrix:

$$S_{12}(\lambda_1, \lambda_2)\hat{S}_{32}(\lambda_3, \lambda_2)\hat{S}_{31}(\lambda_3, \lambda_1) = \hat{S}_{31}(\lambda_3, \lambda_1)\hat{S}_{32}(\lambda_3, \lambda_2)S_{12}(\lambda_1, \lambda_2).$$
(17.15)

We see the important fact that the order of multiplication of two S or \tilde{S} matrices is interchanged by the same intertwiner $S_{12}(\lambda_1, \lambda_2)$.

The quantum transfer matrix (17.12) is equal to the trace in the auxiliary ξ -space of the monodromy matrix $\mathcal{T}_{\xi}(\lambda)$, $T^{\text{QTM}}(\lambda) = \text{Tr}_{\xi} \mathcal{T}_{\xi}(\lambda)$. The monodromy matrix is expressible as the product of N Lax operators

$$\mathcal{T}_{\xi}(\lambda) = \prod_{n=1}^{N/2} \left[L_{\xi,2n-1}(\lambda-\tau) \tilde{L}_{\xi,2n}(\lambda+\tau) \right].$$
(17.16)

Here, the Lax operators at odd sites, corresponding to S, are given in the auxiliary $2 \times 2 \xi$ -space by

$$L_{2n-1}(\lambda) = \begin{pmatrix} w_0(\lambda)\boldsymbol{\sigma}_{2n-1}^0 + w_3(\lambda)\boldsymbol{\sigma}_{2n-1}^z & w_1(\lambda)\boldsymbol{\sigma}_{2n-1}^- \\ w_1(\lambda)\boldsymbol{\sigma}_{2n-1}^+ & w_0(\lambda)\boldsymbol{\sigma}_{2n-1}^0 - w_3(\lambda)\boldsymbol{\sigma}_{2n-1}^z \end{pmatrix}$$
(17.17)

and the ones at even sites, corresponding to \tilde{S} , by

$$\tilde{L}_{2n}(\lambda) = \begin{pmatrix} w_0(-\lambda)\boldsymbol{\sigma}_{2n}^0 + w_3(-\lambda)\boldsymbol{\sigma}_{2n}^z & w_1(-\lambda)\boldsymbol{\sigma}_{2n}^+ \\ w_1(-\lambda)\boldsymbol{\sigma}_{2n}^- & w_0(-\lambda)\boldsymbol{\sigma}_{2n}^0 - w_3(-\lambda)\boldsymbol{\sigma}_{2n}^z \end{pmatrix};$$
(17.18)

the parameters w_0 , w_1 and w_3 are related to the vertex weights as follows $w_0 = (a + b)/2$, $w_1 = c/2$ and $w_3 = (a - b)/2$. The YBEs (17.2) and (17.15) are equivalent to the relations

$$R(\lambda - \mu) [L_{2n-1}(\lambda - \tau) \otimes L_{2n-1}(\mu - \tau)] = [L_{2n-1}(\mu - \tau) \otimes L_{2n-1}(\lambda - \tau)] \times R(\lambda - \mu), \qquad (17.19)$$
$$R(\lambda - \mu) \left[\tilde{L}_{2n}(\lambda + \tau) \otimes \tilde{L}_{2n}(\mu + \tau) \right] = \left[\tilde{L}_{2n}(\mu + \tau) \otimes \tilde{L}_{2n}(\lambda + \tau) \right] \times R(\lambda - \mu), \qquad (17.20)$$

respectively. Here, the ordinary and tensor products are taken in the extended auxiliary (ξ, η) space and $R(\lambda) = \mathcal{P}S(\lambda)$. Since the two kinds of Lax operators are interchanged by the same intertwiner, the monodromy matrix (17.16) satisfies the permutation relation

$$R(\lambda - \mu) \left[\mathcal{T}(\lambda) \otimes \mathcal{T}(\mu) \right] = \left[\mathcal{T}(\mu) \otimes \mathcal{T}(\lambda) \right] R(\lambda - \mu).$$
(17.21)

This immediately leads to the commutation formula $[T^{\text{QTM}}(\lambda), T^{\text{QTM}}(\mu)] = 0$ valid for arbitrary λ and μ .

Having the commuting family of the quantum transfer matrices, we proceed in analogy with Sect. 8.3. Using the representation (8.31) of the monodromy matrix in the ξ -space in the permutation relation (17.21), the permutation relations between the operators $\{A, B, C, D\}$ are the same as in Eqs. (8.34)–(8.36). The action of the Lax operator at an odd site on the spin-up vector e^+ at the same site implies the triangle form

$$L_{2n-1}(\lambda - \tau)e_{2n-1}^{+} = \begin{pmatrix} a(\lambda - \tau) & [\cdots] \\ 0 & b(\lambda - \tau) \end{pmatrix} e_{2n-1}^{+}.$$
(17.22)

The action of the Lax operator at an even site (17.18) on the spin-up vector e^+ leads to a different triangle form, with 0 above the diagonal. This is the problem since only diagonal elements of products of the same-type triangle matrices are available explicitly. The solution of the problem is simple. We have to choose the generating vector Ω as the tensor product of alternating spin-up vectors $e^+ = {0 \choose 1}$ on odd sites and spin-down vectors $e^- = {0 \choose 1}$ on even sites,

$$\Omega = \underbrace{e^+}_1 \otimes \underbrace{e^-}_2 \otimes \cdots \otimes \underbrace{e^+}_{N-1} \otimes \underbrace{e^-}_N.$$
(17.23)

The action of the Lax operator at an even site on the spin-down vector e^- implies the "correct" triangle form

$$L_{2n}(\lambda + \tau)e_{2n}^{-} = \begin{pmatrix} b(-\lambda - \tau) & [\cdots] \\ 0 & a(-\lambda - \tau) \end{pmatrix} e_{2n}^{-}.$$
(17.24)

The monodromy matrix thus acts on the generating vector Ω as follows

$$\mathcal{T}(\lambda)\Omega = \begin{pmatrix} [a(\lambda-\tau)b(-\lambda-\tau)]^{N/2} & [\cdots] \\ 0 & [b(\lambda-\tau)a(-\lambda-\tau)]^{N/2} \end{pmatrix} \Omega.$$
(17.25)

We recall that if the magnetic field $h \neq 0$, the diagonal ++ and -- elements must be multiplied by the Boltzmann factors $e^{\beta h}$ and $e^{-\beta h}$, respectively.

The diagonalization procedure follows the standard QISM and we only write down the final results. In the sector with M spins down, the eigenvalues of the quantum transfer matrix are given by

$$t^{\text{QTM}}(\lambda) = \alpha(\lambda) \prod_{j=1}^{M} \frac{a(\lambda_j - \lambda)}{b(\lambda_j - \lambda)} + \beta(\lambda) \prod_{j=1}^{M} \frac{a(\lambda - \lambda_j)}{b(\lambda - \lambda_j)}.$$
(17.26)

Here, the abbreviations $\alpha(\lambda)$ and $\beta(\lambda)$ are used for the products

$$\alpha(\lambda) = e^{\beta h} [a(\lambda - \tau)b(-\lambda - \tau)]^{N/2}, \qquad \beta(\lambda) = e^{-\beta h} [b(\lambda - \tau)a(-\lambda - \tau)]^{N/2} (17.27)$$

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and $\{\lambda_j\}_{j=1}^M$ are the distinct roots of the Bethe ansatz equations

$$\frac{\alpha(\lambda_j)}{\beta(\lambda_j)} = \prod_{\substack{k=1\\(k\neq j)}}^{M} \left[\frac{a(\lambda_j - \lambda_k)}{a(\lambda_k - \lambda_j)} \frac{b(\lambda_k - \lambda_j)}{b(\lambda_j - \lambda_k)} \right] \qquad j = 1, \dots, M.$$
(17.28)

Since b(0) = 0, the same set of equations is obtained from (17.26) by requiring that $t(\lambda)$ be analytic in the whole complex plane, i.e.

$$\operatorname{Res} t(\lambda = \lambda_j) = 0 \qquad \text{for all } j = 1, \dots, M.$$
(17.29)

We shall rewrite the above equations into a form which is more convenient for a general analysis. We replace $\lambda \to i\lambda$ and $\lambda_j \to i\lambda_j$. Introducing the odd function

$$r(\lambda) = \sinh(\gamma\lambda/2), \qquad r(\lambda) = -r(-\lambda),$$
(17.30)

we express $b(\mathrm{i}\lambda)=r(\lambda)/r(\lambda-2\mathrm{i})$ and

$$\alpha(i\lambda) = e^{\beta h} \left[\frac{r(\lambda - i\tau)}{r(\lambda - i\tau + 2i)} \right]^{N/2}, \qquad \beta(i\lambda) = e^{-\beta h} \left[\frac{r(\lambda + i\tau)}{r(\lambda + i\tau - 2i)} \right]^{N/2}.$$
 (17.31)

For the eigenvalues $\Lambda(\lambda) \equiv t(i\lambda)$, the expression (17.26) can be rewritten as

$$\Lambda(\lambda) = \frac{\Lambda_1(\lambda) + \Lambda_2(\lambda)}{[r(\lambda - i(2 - \tau))r(\lambda + i(2 - \tau))]^{N/2}}$$
(17.32)

with

$$\Lambda_1(\lambda) = e^{\beta h} \phi(\lambda - i) \frac{q(\lambda + 2i)}{q(\lambda)}, \qquad (17.33)$$

$$\Lambda_2(\lambda) = e^{-\beta h} \phi(\lambda + i) \frac{q(\lambda - 2i)}{q(\lambda)}.$$
(17.34)

Here,

$$\phi(\lambda) = [r(\lambda - i(1 - \tau))r(\lambda + i(1 - \tau))]^{N/2}$$
(17.35)

and the function $q(\lambda)$ is defined in terms of the as-yet-undetermined Bethe ansatz roots as follows

$$q(\lambda) = \prod_{j=1}^{M} r(\lambda - \lambda_j).$$
(17.36)

The condition which fixes the values of $\{\lambda_j\}$ is now the analyticity of $\Lambda_1 + \Lambda_2$ in the complex λ -plane. Defining the function

$$a(\lambda) \equiv \frac{\Lambda_1(\lambda)}{\Lambda_2(\lambda)} = e^{2\beta h} \frac{\phi(\lambda - i)q(\lambda + 2i)}{\phi(\lambda + i)q(\lambda - 2i)},$$
(17.37)

the analyticity requirement is equivalent to the condition

$$a(\lambda_j) = -1$$
 $j = 1, \dots, M.$ (17.38)



Fig. 17.1. The function $a(\lambda)$: Distribution of poles (crosses) and zeros (open circles)

17.3 Non-linear integral equations for eigenvalues

In the study of the antiferromagnetic XXZ Hamiltonian, the absolute ground state was determined as the unique solution of the Bethe ansatz equations in the sector $s^z = 0$ (M = N/2) with all N/2 roots being *real*. The corresponding quantum numbers were distributed equidistantly and symmetrically about the origin; as a consequence, the Bethe ansatz roots appeared in conjugate couples $\lambda_j = -\lambda_{N/2-j+1}$. The largest eigenvalue $\Lambda(0)$ of the quantum transfer matrix is determined by an analogous antiferromagnetic state. For $h \neq 0$, the Bethe ansatz roots are complex and possess the symmetries

$$\lambda_j(h) = \bar{\lambda}_j(-h), \qquad \lambda_j(h) = -\bar{\lambda}_{N/2-j+1}(h). \tag{17.39}$$

As $h \rightarrow 0$, the Bethe ansatz roots go continuously to the real values which possess the symmetry of the antiferromagnetic ground state

$$\lambda_j = -\lambda_{N/2-j+1}$$
 $j = 1, \dots, N/2.$ (17.40)

For this specific case we have $q(-\lambda) = (-1)^{N/2}q(\lambda)$ and $\phi(\lambda) = \phi(-\lambda)$, so the a-function (17.37) satisfies the equality

$$a(-\lambda) = \frac{1}{a(\lambda)}.$$
(17.41)

There is a fundamental difference between the Bethe ansatz equations in the study of the eigenvalues of the XXZ Hamiltonian and the present ones. The ratio of ϕ -functions in (17.37) possesses zeros and poles which converge to the real axis in the limit $N \to \infty$. Consequently, the distribution of the Bethe ansatz roots is discrete (roots have spacing of order larger than O(1/N)) for $\lambda > 0$ and exhibits an accumulation point at the origin $\lambda = 0$. Therefore the roots cannot be described by a continuous density as before.

The function $a(\lambda)$ possesses poles and zeros depicted in Fig. 17.1 by crosses and open circles, respectively. For each Bethe ansatz root λ_j , there exists a simple pole at $\lambda_j + 2i$ and a simple



Fig. 17.2. The function $A(\lambda)$: Distribution of poles (crosses) and zeros (open circles correspond to the Bethe ansatz roots, open squares correspond to additional hole-type zeros)

zero at $\lambda_j - 2i$. There are additional poles and zeros at $\pm i\tau$ and $\pm i(2 - \tau)$) which are of order N/2.

We define an auxiliary function $A(\lambda)$ by

$$A(\lambda) = 1 + a(\lambda). \tag{17.42}$$

The poles of this function are equivalent to those of $a(\lambda)$. There are two kinds of zeros, see Fig. 17.2. Due to the equality (17.38), one set is composed of N/2 Bethe ansatz roots (open circles); the positions of these zeros are directly related to those occurring in the function $a(\lambda)$. There are additional N zeros (open squares) far away from the real axis, their imaginary parts being close to $\pm 2i$. They are referred to as hole-type solutions of the Bethe ansatz equations and their importance will be evident later.

Our strategy is to derive an integral equation which relates $\ln a(\lambda)$ and $\ln A(\lambda)$. Let us consider the function

$$g(\lambda) = \frac{1}{2\pi i} \oint_{\Gamma} d\lambda' \frac{d}{d\lambda} \ln r(\lambda - \lambda') \ln A(\lambda'), \qquad (17.43)$$

where the anticlockwise integration in the complex plane is along the closed contour Γ surrounding the real axis, the Bethe ansatz roots $\{\lambda_j\}$ and the point $-i\tau$ (see Fig. 17.2). The number N/2of zeros of $A(\lambda)$ inside this contour is identical to order of pole at $-i\tau$. The integrand $\ln A(\lambda')$ has therefore zero winding number on the contour and the integral is well defined. Integration by parts and the application of the Chauchy theorem to (17.43) yields

$$g(\lambda) = \sum_{j=1}^{N/2} \ln r(\lambda - \lambda_j) - \frac{N}{2} \ln r(\lambda + i\tau) = \ln \frac{q(\lambda)}{r(\lambda + i\tau)^{N/2}}.$$
(17.44)

Combining this equation with the definition (17.37) of $a(\lambda)$, we obtain

$$\ln a(\lambda) = 2\beta h + \frac{N}{2} \ln \left(\frac{r(\lambda - i\tau)r(\lambda + 2i + i\tau)}{r(\lambda + i\tau)r(\lambda + 2i - i\tau)} \right) + g(\lambda + 2i) - g(\lambda - 2i).$$
(17.45)

To simplify the notation, we denote the logarithmic derivative of $r(\lambda)$ as

$$d(\lambda) \equiv \frac{\mathrm{d}}{\mathrm{d}\lambda} \ln r(\lambda) = \frac{\gamma}{2} \coth\left(\frac{\gamma}{2}\lambda\right). \tag{17.46}$$

This function satisfies important equalities

$$d(\lambda + n\mathbf{i}) + d(\lambda - n\mathbf{i}) = \gamma \frac{\sinh(\gamma \lambda)}{\cosh(\gamma \lambda) - \cos(n\gamma)}$$
(17.47)

$$d(\lambda + ni) - d(\lambda - ni) = -i\gamma \frac{\sin(n\gamma)}{\cosh(\gamma\lambda) - \cos(n\gamma)},$$
(17.48)

valid for any real *n*. According to the representation (17.43), the integration kernel κ of the difference $g(\lambda - 2i) - g(\lambda + 2i)$ is given by

$$\kappa(\lambda) = \frac{1}{2\pi i} \frac{d}{d\lambda} \ln \frac{r(\lambda - 2i)}{r(\lambda + 2i)} = \frac{1}{2\pi i} \left[d(\lambda - 2i) - d(\lambda + 2i) \right]$$
$$= \frac{\gamma}{2\pi} \frac{\sin(2\gamma)}{\cosh(\gamma\lambda) - \cos(2\gamma)}.$$
(17.49)

The Trotter number N enters only the first term on the rhs of (17.45), which has the well defined $N \rightarrow \infty$ limit:

$$\lim_{N \to \infty} \frac{N}{2} \ln \left(\frac{r(\lambda - i\tau)r(\lambda + 2i + i\tau)}{r(\lambda + i\tau)r(\lambda + 2i - i\tau)} \right) \sim Ni\tau \left[\frac{d}{d\lambda} \ln r(\lambda + 2i) - \frac{d}{d\lambda} \ln r(\lambda) \right]$$
$$= i\beta 2 \frac{\sin \gamma}{\gamma} \left[d(\lambda + 2i) - d(\lambda) \right]. \quad (17.50)$$

Thus in the limit $N \to \infty$ Eq. (17.45) becomes the non-linear integral equation (NLIE) for $a(\lambda)$

$$\ln a(\lambda) = 2\beta h + \beta \epsilon_0(\lambda + i) - \oint_{\Gamma} d\lambda' \kappa(\lambda - \lambda') \ln A(\lambda'), \qquad (17.51)$$

where $\epsilon_0(\lambda)$ is defined by

$$\epsilon_0(\lambda) = i2 \frac{\sin \gamma}{\gamma} \left[d(\lambda + i) - d(\lambda - i) \right] = 2 \frac{\sin^2 \gamma}{\cosh(\gamma \lambda) - \cos \gamma}.$$
(17.52)

There are other variants of this NLIE which are more convenient for low temperatures. Let us consider the function $a(\lambda)$ on the axes $Im(\lambda) = \pm 1$, the integration contour Γ is chosen just below and above these axes. Writing Eq. (17.51) for $\lambda = x - i$ ($x \in \mathbb{R}$), we make the following "particle-hole" transformation on the lower part of Γ :

$$a(x-i) = \frac{1}{\bar{a}(x-i)}, \qquad \ln A(x-i) = \ln \bar{A}(x-i) - \ln \bar{a}(x-i), \qquad (17.53)$$

where $\bar{A} = 1 + \bar{a}$. The resulting equation contains convolution integrals with $\ln A$, $\ln \bar{A}$ and \bar{a} . It can be formally solved for $\bar{b}(x) \equiv \bar{a}(x - i)$ in the Fourier space by using the convolution

theorem. Then, Eq. (17.51) taken at $\lambda = x + i$ can be solved for $b(x) \equiv a(x + i)$. The final coupled set of NLIEs for the new functions reads

$$\ln \mathbf{b}(x) = -\frac{\sin \gamma}{\gamma} \frac{\pi \beta}{\cosh(\pi x/2)} + \frac{\pi \beta h}{\pi - \gamma} + p * \ln \mathbf{B}(x) - p * \ln \bar{\mathbf{B}}(x + 2\mathbf{i}), \quad (17.54)$$

$$\ln \bar{\mathbf{b}}(x) = -\frac{\sin \gamma}{\gamma} \frac{\pi \beta}{\cosh(\pi x/2)} - \frac{\pi \beta h}{\pi - \gamma} + p * \ln \bar{\mathbf{B}}(x) - p * \ln \mathbf{B}(x - 2\mathbf{i}), \quad (17.55)$$

where

$$B(x) = 1 + b(x), \qquad \bar{B}(x) = 1 + \bar{b}(x),$$
(17.56)

the function p(x) is given by

$$p(x) = \int_{-\infty}^{\infty} \frac{\mathrm{d}k}{2\pi} \frac{\sinh\left(\frac{\pi}{\gamma} - 2\right)k}{2\cosh k \sinh\left(\frac{\pi}{\gamma} - 1\right)k} \mathrm{e}^{\mathrm{i}kx}$$
(17.57)

and the integration paths are well defined just below or above real axis.

For h = 0 with all N/2 "antiferromagnetic" Bethe roots being real numbers, the above procedure can be applied to the integration contour Γ whose lower part goes just below and the upper part just above the real axis. The result is the single NLIE of the form

$$-i\ln a(x) = -\frac{\sin\gamma}{\gamma} \frac{\pi\beta}{\sinh(\pi x/2)} + 2\int_{-\infty}^{\infty} dx' \, p(x-x') \mathrm{Im} \, \ln[1 + a(x'+i0)].$$
(17.58)

17.4 Representations of the free energy

The next step is to express the QTM eigenvalues $\Lambda(\lambda)$ in terms of the quantities determined in the previous part by integral equations.

We start with the derivation of an integral expression for $\Lambda(\lambda)$ in terms of $a(\lambda)$ or $A(\lambda)$, satisfying the integral equation (17.51). As follows from Eqs. (17.32)–(17.38), the sum $\Lambda_1(\lambda) + \Lambda_2(\lambda)$ is an analytic function of λ , periodic along the imaginary axis with period $2\pi i/\gamma$ and with exponential asymptotic along the real axis. This is why we can write

$$\Lambda_1(\lambda) + \Lambda_2(\lambda) = C \prod_{j=1}^N r(\lambda - \mu_j), \qquad (17.59)$$

where C is a constant and $\{\mu_j\}_{j=1}^N$ are the hole-type zeros of $A(\lambda) = 1 + a(\lambda)$, $a(\lambda) = \Lambda_1(\lambda)/\Lambda_2(\lambda)$. These zeros, which are not the Bethe ansatz roots, are localized close to the $\pm 2i$ axes and depicted by open squares in Fig.17.2.

As before, let Γ be a closed contour which surrounds the real axis, the Bethe ansatz roots $\{\lambda_j\}$ and the point $-i\tau$, but not the hole-type zeros $\{\mu_j\}$. For λ close to the real axis, the application of the Cauchy theorem yields

$$\frac{1}{2\pi \mathrm{i}} \oint_{\Gamma} \mathrm{d}\lambda' \, d(\lambda - \lambda' - 2\mathrm{i}) \frac{\mathrm{d}}{\mathrm{d}\lambda'} \ln \mathcal{A}(\lambda') = \sum_{j=1}^{N/2} d(\lambda - \lambda_j - 2\mathrm{i}) - \frac{N}{2} d(\lambda + \mathrm{i}\tau - 2\mathrm{i}).(17.60)$$

We also have

$$\frac{1}{2\pi i} \oint_{\Gamma} d\lambda' \, d(\lambda - \lambda') \frac{d}{d\lambda'} \ln A(\lambda') = \sum_{j=1}^{N/2} d(\lambda - \lambda_j - 2i) - \sum_{j=1}^{N} d(\lambda - \mu_j) + \frac{N}{2} d(\lambda + 2i - i\tau).$$
(17.61)

Here, we replaced the contour Γ by a new contour $\tilde{\Gamma}$, such that its upper part is the lower part of Γ and its lower part is the upper part of Γ shifted by the period $-2\pi i/\gamma$, reversing orientation. The surrounded singularities of the integrand are poles and zeros of the A-function: There are N/2 simple poles at $\lambda_j + 2i - 2\pi i/\gamma$, N zeros at μ_j (one half with and the other half without shift $-2\pi i/\gamma$) and one pole of order N/2 at $i\tau - 2i$. Subtracting Eqs. (17.60) and (17.61), integrating by parts and finally integrating with respect to λ , we obtain

$$\frac{1}{2\pi i} \oint_{\Gamma} d\lambda' \left[d(\lambda - \lambda') - d(\lambda - \lambda' - 2i) \right] \ln A(\lambda')$$
$$= \ln \frac{\left[r(\lambda - i(2 - \tau))r(\lambda + i(2 - \tau)) \right]^{N/2}}{\prod_{j} r(\lambda - \mu_{j})} + \text{const.}$$
(17.62)

In view of (17.32) and (17.59), this relation gives

$$\ln \Lambda(\lambda) = -\beta h - \frac{1}{2\pi i} \oint_{\Gamma} d\lambda' \left[d(\lambda - \lambda') - d(\lambda - \lambda' - 2i) \right] \ln A(\lambda').$$
(17.63)

The constant is fixed by the asymptotic formulas $\Lambda(\infty) = \exp(\beta h) + \exp(-\beta h)$ and $A(\infty) = 1 + \exp(2\beta h)$.

We proceed with the derivation of an integral expression for Λ in terms of B(x) and $\overline{B}(x)$, given by Eqs. (17.54)–(17.57). Λ_1 can be eliminated from (17.32) via $\Lambda_1(\lambda) = a(\lambda)\Lambda_2(\lambda)$. Taking $\lambda = x + i$ with $x \in \mathbb{R}$, we get

$$\Lambda(x+i) = e^{-\beta h} \left[\frac{r(x+i(1+\tau))}{r(x-i(1-\tau))} \right]^{N/2} \frac{q(x-i)}{q(x+i)} B(x).$$
(17.64)

Similarly, Λ_2 can be eliminated from (17.32) via $\Lambda_2(\lambda) = \lambda_1(\lambda)/a(\lambda)$. Taking $\lambda = x - i$, we get

$$\Lambda(x - i) = e^{\beta h} \left[\frac{r(x - i(1 + \tau))}{r(x + i(1 - \tau))} \right]^{N/2} \frac{q(x + i)}{q(x - i)} \bar{B}(x).$$
(17.65)

The multiplication of Eqs. (17.64) and (17.65) results in the "inversion identity"

$$\Lambda(x+i)\Lambda(x-i) = \left[\frac{r(x+i(1+\tau))r(x-i(1+\tau))}{r(x-i(1-\tau))r(x+i(1-\tau))}\right]^{N/2} B(x)\bar{B}(x)$$
(17.66)

which no longer involves the q-function. Taking the logarithm of this equation, we find in the limit $N \to \infty$ that

$$\ln \Lambda(x+\mathbf{i}) + \ln \Lambda(x-\mathbf{i}) = \beta \epsilon_0(x) + \ln[\mathbf{B}(x)\overline{\mathbf{B}}(x)].$$
(17.67)

The solution, obtained by the Fourier transform, at x = 0 reads

$$\ln \Lambda(0) = -\beta e_0 + \int_{-\infty}^{\infty} \mathrm{d}x \, \frac{1}{4\cosh(\pi x/2)} \ln[\mathbf{B}(x)\bar{\mathbf{B}}(x)],\tag{17.68}$$

where e_0 is the ground state energy per site of the XXZ chain.

For the special case h = 0, the formula for $\Lambda(0)$ in terms of a(x), satisfying (17.58), can be derived in a similar way. The final result is

$$\ln \Lambda(0) = -\beta e_0 - \operatorname{Im} \int_{-\infty}^{\infty} \mathrm{d}x \, \frac{1}{2\sinh[\pi(x+\mathrm{i}0)/2]} \ln[1 + \mathrm{a}(x+\mathrm{i}0)]. \tag{17.69}$$

17.5 High-temperature expansion

We construct the high-temperature asymptotic expansion of the free energy f by using the function $a(\lambda)$, which satisfies the integral equation (17.51).

For $\beta \to 0$, the function $a(\lambda)$ becomes independent of λ since the integrand in (17.51) has no poles in the area surrounded by the contour Γ . Inserting the result $a(\lambda) \sim 1$ into the integral in (17.63) leads to the correct high-temperature entropy $-\beta f = \ln \Lambda(0) \sim \ln 2$.

For small values of β , we search $a(\lambda)$ as the series expansion

$$a(\lambda) = e^{-iz(\lambda)}, \qquad z(\lambda) = \beta z_1(\lambda) + \beta^2 z_2(\lambda) + \cdots.$$
(17.70)

With regard to the expansion formula

$$\ln\left[1 + e^{-iz}\right] = \ln 2 - \frac{i\beta}{2}z_1 - \frac{\beta^2}{2}\left[iz_2 + \frac{1}{4}z_1^2\right] + \cdots,$$
(17.71)

the integral equation (17.51) transforms itself into an infinite sequence of coupled equations for the expansion functions $\{z_i(\lambda)\}$:

$$z_1(\lambda) = 2ih + i\epsilon_0(\lambda + i) - \frac{1}{2} \oint_{\Gamma} d\lambda' \kappa(\lambda - \lambda') z_1(\lambda'), \qquad (17.72)$$

$$z_2(\lambda) = -\frac{1}{2i} \oint_{\Gamma} d\lambda' \,\kappa(\lambda - \lambda') \left[i z_2(\lambda') + \frac{1}{4} z_1^2(\lambda') \right], \qquad (17.73)$$

etc. The second term on the rhs of (17.72) causes that $z_1(\lambda)$ has a simple pole at the origin,

$$z_1(\lambda) \underset{\lambda \to 0}{\sim} \frac{2\sin\gamma}{\gamma} \frac{1}{\lambda}.$$
(17.74)

This is the only pole of $z_1(\lambda)$ inside the contour Γ and the application of the residue theorem implies

$$z_1(\lambda) = 2ih - \sin\gamma \left[\frac{\sinh(\gamma\lambda)}{\cosh(\gamma\lambda) - \cos(2\gamma)} - \coth\left(\frac{\gamma\lambda}{2}\right) \right].$$
(17.75)

It turns out that in the whole infinite sequence of equations only the poles at $\lambda = 0$ contribute to the contour integral over Γ . All the $z_j(\lambda)$ with $j \ge 2$ are analytic there. This makes the procedure of finding the expansion functions simply recursive. For $z_2(\lambda)$, we find

$$z_2(\lambda) = -2\frac{\sin\gamma\sin(2\gamma)}{\cosh(\gamma\lambda) - \cos(2\gamma)} \left[2ih + \sin\gamma\frac{\sinh(\gamma\lambda)}{\cosh(\gamma\lambda) - \cos(2\gamma)} \right],$$
(17.76)

etc.

Finally, we insert the expansion functions $\{z_j(\lambda)\}\$ into the formula (17.63) and apply once again the residuum theorem for simple and higher-order poles at the origin generated by powers of $z_1(\lambda)$. The high-temperature expansion of the free energy is obtained in form

$$-\beta f = \ln 2 + \frac{\beta}{2}\cos\gamma + \frac{\beta^2}{4}\left[\left(1 + \frac{1}{2}\cos^2\gamma\right) + 2h^2\right] + O(\beta^3).$$
 (17.77)

For $\gamma = 0$, this expansion is in agreement with the antiferromagnetic J = -1 high-temperature result (16.55) derived directly from the cumulant expansion of the free energy.

17.6 Low-temperature expansion

For h = 0, we construct the low-temperature expansion of the free energy f by using the function a(x), satisfying the NLIE (17.58).

In the low-temperature limit $\beta \to \infty$, the leading corrections to the ground state quantities come from absolute values of x larger than

$$\xi = \frac{2}{\pi} \ln \left(2\pi\beta \frac{\sin\gamma}{\gamma} \right). \tag{17.78}$$

It is convenient to introduce the scaling functions

$$\mathbf{a}_{\xi}(x) \equiv \mathbf{a}(x+\xi), \qquad \tilde{\mathbf{a}}_{\xi}(x) \equiv \mathbf{a}(-x-\xi). \tag{17.79}$$

They approach well-defined functions in the low-temperature limit which satisfy

$$- i \ln a_{\xi}(x) = -e^{-\pi x/2} + 2 \int_{-\infty}^{\infty} dx' \, p(x - x') \operatorname{Im} \ln \left[1 + a_{\xi}(x' + i0) \right], \quad (17.80)$$

$$-i\ln\tilde{a}_{\xi}(x) = e^{-\pi x/2} + 2\int_{-\infty}^{\infty} dx' \, p(x-x') \operatorname{Im} \ln\left[1 + \tilde{a}_{\xi}(x'-i0)\right].$$
(17.81)

The h = 0 equality (17.41) implies $a_{\xi}(x) = 1/\tilde{a}_{\xi}(x)$. In view of the above integral equations, this is equivalent to the relation

$$\operatorname{Im} \ln \left[1 + a_{\xi}(x + i0)\right] = -\operatorname{Im} \ln \left[1 + \tilde{a}_{\xi}(x - i0)\right]$$
(17.82)

valid for any $x \in (-\infty, \infty)$.

In the integral of the eigenvalue representation (17.69), we make the substitutions $x = x' + \xi$ for x > 0 and $x = -x' - \xi$ for x < 0, to obtain

$$\int_{-\infty}^{\infty} dx \frac{1}{2\sinh[\pi(x+i0)/2]} \ln[1+a(x+i0)]$$

$$= \int_{-\xi}^{\infty} dx' \frac{1}{2\sinh[\pi(x'+\xi+i0)/2]} \ln[1+a_{\xi}(x'+i0)]$$

$$- \int_{-\xi}^{\infty} dx' \frac{1}{2\sinh[\pi(x'+\xi-i0)/2]} \ln[1+\tilde{a}_{\xi}(x'-i0)].$$
(17.83)

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With respect to the equality (17.82), in the limit $\beta \rightarrow \infty$ we find

$$\ln \Lambda(0) = -\beta e_0(\gamma) - \frac{\gamma}{\pi\beta \sin \gamma} \operatorname{Im} \int_{-\infty}^{\infty} \mathrm{d}x \, \mathrm{e}^{-\pi x/2} \ln[1 + \mathrm{a}_{\xi}(x + \mathrm{i}0)] + O(\beta^{-2}).(17.84)$$

The integral in (17.84) can be evaluated by using the following lemma [35, 36]. Let F(x) satisfies the NLIE

$$-i\ln F(x) = \varphi(x) + 2\int_{x_1}^{x_2} dy \, p(x-y) \text{Im} \, \ln\left[1 + F(y+i0)\right], \tag{17.85}$$

where $\varphi(x)$ is a real function for real x and x_1, x_2 are real numbers. Then the following equality holds

$$\operatorname{Im} \int_{x_1}^{x_2} \mathrm{d}x \, \varphi'(x) \ln[1 + F(x + \mathrm{i0})] = \frac{1}{2} \operatorname{Re} \left[l(F_1) - l(F_2) \right] \\ + \frac{1}{2} \left[\varphi(x_2) \operatorname{Im} \ln(1 + F_2) - \varphi(x_1) \operatorname{Im} \ln(1 + F_1) \right] \\ + \int_{x_1}^{x_2} \mathrm{d}y \left[p(x_2 - y) \operatorname{Im} \ln(1 + F_2) - p(x_1 - y) \operatorname{Im} \ln(1 + F_1) \right] \\ \times \operatorname{Im} \ln \left[1 + F(y + \mathrm{i0}) \right],$$
(17.86)

where $F_{1,2} \equiv F(x_{1,2})$ and l(t) is a dilogarithm function

$$l(t) \equiv \int_0^t du \left[\frac{\ln(1+u)}{u} - \frac{\ln u}{1+u} \right].$$
 (17.87)

The proof of the lemma starts from the relation

$$l(F_{2}) - l(F_{1}) = \int_{F_{1}}^{F_{2}} du \left[\frac{\ln(1+u)}{u} - \frac{\ln u}{1+u} \right]$$

$$= \int_{x_{1}}^{x_{2}} dx \left\{ \ln \left[1 + F(x+i0) \right] \frac{d}{dx} \ln F(x) - \ln F(x) \frac{d}{dx} \ln \left[1 + F(x+i0) \right] \right\},$$
(17.88)

obtained by using the substitution u = F(x). We substitute $\ln F(x)$ and $d \ln F(x)/dx$ by using Eq. (17.85) and its derivative, respectively. The result is

$$l(F_{2}) - l(F_{1}) = i \int_{x_{1}}^{x_{2}} dx \left\{ \varphi'(x) \ln \left[1 + F(x + i0)\right] - \varphi(x) \frac{d}{dx} \ln \left[1 + F(x + i0)\right] \right\}$$

+2i $\int_{x_{1}}^{x_{2}} dx \int_{x_{1}}^{x_{2}} dy \left\{ \ln \left[1 + F(x + i0)\right] p'(x - y) - p(x - y) \frac{d}{dx} \ln \left[1 + F(x + i0)\right] \right\} \operatorname{Im} \ln \left[1 + F(y + i0)\right].$ (17.89)

The second terms in the simple and double integrals are integrated by parts. Taking then real part of both sides, the double integral

$$\int_{x_1}^{x_2} \mathrm{d}x \int_{x_1}^{x_2} \mathrm{d}y \, p'(x-y) \mathrm{Im} \, \ln\left[1 + F(x+\mathrm{i0})\right] \mathrm{Im} \, \ln\left[1 + F(y+\mathrm{i0})\right]$$

vanishes due to the relation p'(x - y) = -p'(y - x). We end up with (17.86).

Choosing $F(x) = a_{\xi}(x)$, from (17.80) we have $\varphi(x) = -\exp(-\pi x/2)$ and $x_1 = -\infty$, $x_2 = \infty$. Since $F(x_1) = 0$, $F(x_2) = 0$, the formula (17.86) fixes the value of the integral

$$\operatorname{Im} \int_{-\infty}^{\infty} \mathrm{d}x \,\mathrm{e}^{-\pi x/2} \ln\left[1 + \mathrm{a}_{\xi}(x + \mathrm{i}0)\right] = -\frac{2}{\pi} \frac{1}{2} l(1) = -\frac{\pi}{6}.$$
(17.90)

From (17.84) we finally obtain

$$f(T, h = 0) = e_0(\gamma) - \frac{\gamma}{6\sin\gamma}T^2 + o(T^2).$$
(17.91)

For the isotropic antiferromagnet $\gamma \rightarrow 0$, we recover the previous result (16.115). At low temperature and h = 0, the specific heat is given by

$$C = \frac{\gamma}{3\sin\gamma}T + o(T). \tag{17.92}$$

According to (15.81), the velocity of sound for the paramagnet with $\Delta = -\cos \gamma$ is $v_s = \pi \sin \gamma / \gamma$. Comparing (17.91) with the general formula (16.117) confirms that the central charge c = 1 in the whole paramagnetic region $-1 \le \Delta < 1$.
18 XYZ Heisenberg chain

The XYZ Heisenberg spin chain was solved by Baxter [14, 15]. Using the link between the XYZ spin chain and the eight-vertex model, he obtained a system of transcendental equations for the eigenvalues of the transfer matrix for the eight-vertex model. The ground-state energy of the XYZ chain was evaluated. A generalization of the Bethe ansatz method enabled him to determine also the eigenvectors and eigenvalues of the XYZ model [42–44]. Low-lying excitations were studied in Ref. [45,46]. The thermodynamics was derived in [25,28] by using strings and in [38] without using strings. The method was put into the framework of the QISM in [47].

Here, we review the application of the QISM and describe the ground state of the XYZ model. Low-lying excitations and the thermodynamics can be derived in analogy with the XXZ model, a complication is the manipulation with elliptic functions.

18.1 Diagonalization of the transfer matrix for eight-vertex model

In Sect. 7, we derived the scattering S-matrix which is a two-state solution of the YBE with the elliptic parametrization of entries:

$$S(\lambda) = \begin{pmatrix} a(\lambda) & 0 & 0 & d(\lambda) \\ 0 & b(\lambda) & c(\lambda) & 0 \\ 0 & c(\lambda) & b(\lambda) & 0 \\ d(\lambda) & 0 & 0 & a(\lambda) \end{pmatrix}, \qquad \begin{aligned} a(\lambda) &= & \Theta(\eta)\Theta(\lambda)H(\lambda+\eta) \\ b(\lambda) &= & \Theta(\eta)H(\lambda)\Theta(\lambda+\eta) \\ c(\lambda) &= & H(\eta)\Theta(\lambda)\Theta(\lambda+\eta) \\ d(\lambda) &= & H(\eta)H(\lambda)H(\lambda+\eta) \end{aligned}$$
(18.1)

where $H(\lambda) \equiv H(\lambda, k)$ and $\Theta(\lambda) \equiv \Theta(\lambda, k)$ are the Jacobi theta functions with modulus k. It has been shown in Sect. 8 that the commuting families of transfer matrices constructed from these S-matrix elements correspond to local statistical weights of certain two-dimensional classical vertex models. When the modulus k tends to zero, we have the six-vertex model with the trigonometric parametrization of elements and $d(\lambda) = 0$. The diagonalization of the trigonometric transfer matrix was straightforward within the QISM.

If $d(\lambda) \neq 0$ (the eight-vertex model), the Hilbert subspace of the spin chain with constant S_{tot}^z is not invariant with respect to the Hamiltonian. This prevents from a simple extention of the analytic Bethe ansatz from the six-vertex model. The present strategy of the algebraic Bethe ansatz is to make the texture of the S-matrix (18.1) similar to that of the six-vertex model by a change of the usual spin up and down orthonormal basis $e^+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, e^- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. It is surprising that this problem admits an infinite number of solutions. Let us introduce the covariant vector basis which depends on the spectral parameter λ and is labeled by an integer index $l \in \mathbb{Z}$:

$$X_l(\lambda) = \begin{pmatrix} H(s+\eta(l-1/2)-\lambda)\\ \Theta(s+\eta(l-1/2)-\lambda) \end{pmatrix},$$
(18.2)

$$Y_{l}(\lambda) = \frac{1}{g(\tau_{2l})} \begin{pmatrix} H(t+\eta(l+1/2)+\lambda) \\ \Theta(t+\eta(l+1/2)+\lambda) \end{pmatrix}.$$
(18.3)

Here, s, t are free parameters and

$$g(u) = H(u)\Theta(u), \qquad \tau_l = \frac{s+t}{2} - K + \frac{1}{2}\eta l$$
 (18.4)

with $K \equiv K(k)$. The contravariant vectors X_l^{\dagger} and Y_l^{\dagger} are given by

$$X_{l}^{\dagger}(\lambda) = \left(-\Theta(s+\eta(l-1/2)-\lambda), H(s+\eta(l-1/2)-\lambda)\right),$$
(18.5)

$$Y_l^{\dagger}(\lambda) = \frac{1}{g(\tau_{2l})} \Big(\Theta(t + \eta(l + 1/2) + \lambda), -H(t + \eta(l + 1/2) + \lambda) \Big).$$
(18.6)

For the permuted matrix $R(\lambda, \mu) = \mathcal{P}S(\lambda - \mu)$, the following relations hold

$$R(\lambda,\mu)\left[X_{l}(\lambda)\otimes X_{l+1}(\mu)\right] = h(\lambda-\mu+\eta)\left[X_{l}(\mu)\otimes X_{l+1}(\lambda)\right],$$
(18.7)

$$R(\lambda,\mu)\left[Y_{l+1}(\lambda)\otimes Y_{l}(\mu)\right] = h(\lambda-\mu+\eta)\left[Y_{l+1}(\mu)\otimes Y_{l}(\lambda)\right],$$
(18.8)

$$R(\lambda,\mu) \left[Y_{k}(\lambda) \otimes X_{l}(\mu) \right] = \frac{h(\eta)g(\lambda - \mu + \tau_{k+l+1})}{g(\tau_{k+l+1})} \left[Y_{k}(\mu) \otimes X_{l}(\lambda) \right] \\ + \frac{h(\lambda - \mu)g(\tau_{k+l-1})}{g(\tau_{k+l+1})} \frac{g(\tau_{2(k+1)})}{g(\tau_{2k})} \left[X_{l+1}(\mu) \otimes Y_{k+1}(\lambda) \right], \quad (18.9)$$

$$R(\lambda,\mu) \left[X_k(\lambda) \otimes Y_l(\mu) \right] = \frac{h(\eta)g(\mu - \lambda + \tau_{k+l-1})}{g(\tau_{k+l-1})} \left[X_k(\mu) \otimes Y_l(\lambda) \right] \\ + \frac{h(\lambda - \mu)g(\tau_{k+l-1})}{g(\tau_{k+l-1})} \frac{g(\tau_{2(l-1)})}{g(\tau_{2l})} \left[Y_{l-1}(\mu) \otimes X_{k-1}(\lambda) \right], \quad (18.10)$$

where

$$h(u) = \Theta(0)g(u) = \Theta(0)H(u)\Theta(u), \qquad h(-u) = -h(u).$$
 (18.11)

The derivation of these formulas is based on the following addition theorems for the Jacobi theta functions

$$\Theta(u)\Theta(v)H(w)H(u+v+w) + H(u)H(v)\Theta(w)\Theta(u+v+w)$$

= $\Theta(0)\Theta(u+v)H(u+w)H(v+w),$ (18.12)
 $a(u-K)a(v)$

$$H(u-v)\Theta(u+v) - \Theta(u-v)H(u+v) = 2\frac{g(u-K)g(v)}{g(K)}.$$
(18.13)

Similar formulas hold for the contravariant vectors:

$$\begin{bmatrix} Y_l^{\dagger}(\mu) \otimes Y_{l+1}^{\dagger}(\lambda) \end{bmatrix} R(\lambda, \mu) = h(\lambda - \mu + \eta) \begin{bmatrix} Y_l^{\dagger}(\lambda) \otimes Y_{l+1}^{\dagger}(\mu) \end{bmatrix},$$
(18.14)

$$\left[X_{l+1}^{\dagger}(\mu) \otimes X_{l}^{\dagger}(\lambda)\right] R(\lambda,\mu) = h(\lambda-\mu+\eta) \left[X_{l+1}^{\dagger}(\lambda) \otimes X_{l}^{\dagger}(\mu)\right],$$
(18.15)

$$\begin{bmatrix} X_{k}^{\dagger}(\mu) \otimes Y_{l}^{\dagger}(\lambda) \end{bmatrix} R(\lambda,\mu) = \frac{h(\eta)g(\lambda-\mu+\tau_{k+l+1})}{g(\tau_{k+l+1})} \begin{bmatrix} X_{k}^{\dagger}(\lambda) \otimes Y_{l}^{\dagger}(\mu) \end{bmatrix}$$
$$+ \frac{h(\lambda-\mu)g(\tau_{k+l-1})}{g(\tau_{k+l+1})} \frac{g(\tau_{2(l+1)})}{g(\tau_{2l})} \begin{bmatrix} Y_{l+1}^{\dagger}(\lambda) \otimes X_{k+1}^{\dagger}(\mu) \end{bmatrix}, (18.16)$$
$$\begin{bmatrix} Y_{k}^{\dagger}(\mu) \otimes X_{l}^{\dagger}(\lambda) \end{bmatrix} R(\lambda,\mu) = \frac{h(\eta)g(\mu-\lambda+\tau_{k+l-1})}{g(\tau_{k+l-1})} \begin{bmatrix} Y_{k}^{\dagger}(\lambda) \otimes X_{l}^{\dagger}(\mu) \end{bmatrix}$$
$$+ \frac{h(\lambda-\mu)g(\tau_{k+l+1})}{g(\tau_{k+l-1})} \frac{g(\tau_{2(k-1)})}{g(\tau_{2k})} \begin{bmatrix} X_{l-1}^{\dagger}(\lambda) \otimes Y_{k-1}^{\dagger}(\mu) \end{bmatrix}. (18.17)$$

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We see that in the new basis the nonvanishing entries of the R-matrix reproduce the six-vertex texture.

The similarity (gauge) transformation related to the change of basis is described by the 2×2 matrix

$$M_l(\lambda) = (X_l(\lambda), Y_l(\lambda)) \tag{18.18}$$

and by its inverse

$$M_l^{-1}(\lambda) = \frac{1}{\text{Det } M_l(\lambda)} \begin{pmatrix} Y_l^{\dagger}(\lambda) \\ X_l^{\dagger}(\lambda) \end{pmatrix}.$$
(18.19)

As follows from the addition theorem (18.12), the determinant

Det
$$M_l(\lambda) = \frac{2}{g(K)}g\left(\lambda + \frac{t-s+\eta}{2}\right) \equiv m(\lambda)$$
 (18.20)

does not depend on l.

The monodromy matrix of the eight-vertex model \mathcal{T} is equal to the product of Lax operators in the auxiliary ξ -space, see Eq. (7.46). The ordering of Lax operators from left to right, $L_1L_2\cdots L_N$ can be changed to the opposite one, $L_NL_{N-1}\cdots L_1$; as was shown in Sect. 9, this change in the definition of \mathcal{T} has no effect on the spectrum of its trace, i.e. the transfer matrix. We shall use the standard representation in the studied topic

$$\mathcal{T}(\lambda) = L_N(\lambda)L_{N-1}(\lambda)\cdots L_2(\lambda)L_1(\lambda).$$
(18.21)

The Lax operators are given by

$$L_n(\lambda) = \begin{pmatrix} w_0(\lambda)\boldsymbol{\sigma}_n^0 + w_3(\lambda)\boldsymbol{\sigma}_n^3 & w_1(\lambda)\boldsymbol{\sigma}_n^1 - \mathrm{i}w_2(\lambda)\boldsymbol{\sigma}_n^2 \\ w_1(\lambda)\boldsymbol{\sigma}_n^1 + \mathrm{i}w_2(\lambda)\boldsymbol{\sigma}_n^2 & w_0(\lambda)\boldsymbol{\sigma}_n^0 - w_3(\lambda)\boldsymbol{\sigma}_n^3 \end{pmatrix},$$
(18.22)

where the w-functions are expressed in terms of the vertex weights in Eq. (7.57). We consider the following gauge transformation of Lax operators

$$L_n^l(\lambda) = M_{n+l}^{-1}(\lambda)L_n(\lambda)M_{n+l-1}(\lambda) \equiv \begin{pmatrix} \alpha_n^l(\lambda) & \beta_n^l(\lambda) \\ \gamma_n^l(\lambda) & \delta_n^l(\lambda) \end{pmatrix},$$
(18.23)

where l is an integer. The corresponding monodromy matrix

$$\mathcal{T}^{l}(\lambda) = L_{N}^{l}(\lambda)L_{N-1}^{l}(\lambda)\cdots L_{2}^{l}(\lambda)L_{1}^{l}(\lambda)$$
(18.24)

is related to the original one (18.21) by

$$\mathcal{T}^{l}(\lambda) = M_{N+l}^{-1}(\lambda)\mathcal{T}(\lambda)M_{l}(\lambda).$$
(18.25)

It is useful to introduce a family of monodromy matrices $\mathcal{T}_{k,l}$ with integer k, l which are related to the original \mathcal{T} as follows

$$\mathcal{T}_{k,l}(\lambda) = M_k^{-1}(\lambda)\mathcal{T}(\lambda)M_l(\lambda) \equiv \begin{pmatrix} A_{k,l}(\lambda) & B_{k,l}(\lambda) \\ C_{k,l}(\lambda) & D_{k,l}(\lambda) \end{pmatrix}.$$
(18.26)

Here,

$$A_{k,l}(\lambda) = \frac{1}{m(\lambda)} Y_k^{\dagger}(\lambda) \mathcal{T}(\lambda) X_l(\lambda),$$

$$B_{k,l}(\lambda) = \frac{1}{m(\lambda)} Y_k^{\dagger}(\lambda) \mathcal{T}(\lambda) Y_l(\lambda),$$

$$C_{k,l}(\lambda) = \frac{1}{m(\lambda)} X_k^{\dagger}(\lambda) \mathcal{T}(\lambda) X_l(\lambda),$$

$$D_{k,l}(\lambda) = \frac{1}{m(\lambda)} X_k^{\dagger}(\lambda) \mathcal{T}(\lambda) Y_l(\lambda).$$
(18.27)

The family involves the gauge-transformed monodromy matrix (18.24), $\mathcal{T}^{l}(\lambda) = \mathcal{T}_{L+l,l}(\lambda)$. The original transfer matrix T is expressible as

$$T(\lambda) = \operatorname{Tr} \mathcal{T}(\lambda) = \operatorname{Tr} M_l^{-l}(\lambda) \mathcal{T}(\lambda) M_l(\lambda) = A_{l,l}(\lambda) + D_{l,l}(\lambda).$$
(18.28)

The algebra of the operators (18.27) can be derived from the YBE for the original monodromy matrix

$$R(\lambda,\mu)\left[\mathcal{T}(\lambda)\otimes\mathcal{T}(\mu)\right] = \left[\mathcal{T}(\mu)\otimes\mathcal{T}(\lambda)\right]R(\lambda,\mu).$$
(18.29)

Multiplying both sides of this equation from the left by $Y_k^{\dagger}(\mu) \otimes Y_{k+1}^{\dagger}(\lambda)/[m(\lambda)m(\mu)]$ and from the right by $Y_{l+1}(\lambda) \otimes Y_j(\mu)$ and using Eqs. (18.8), (18.14), we find for all integer values of k and l

$$B_{k,l+1}(\lambda)B_{k+1,l}(\mu) = B_{k,l+1}(\mu)B_{k+1,l}(\lambda).$$
(18.30)

A series of similar relations can be derived by applying various combinations of the tensor products of the basis vectors. We shall need the following permutation relations

$$A_{k,l}(\lambda)B_{k+1,l-1}(\mu) = \alpha(\lambda - \mu)B_{k,l-2}(\mu)A_{k+1,l-1}(\lambda) -\beta_{l-1}(\lambda - \mu)B_{k,l-2}(\lambda)A_{k+1,l-1}(\mu),$$
(18.31)

$$D_{k,l}(\lambda)B_{k+1,l-1}(\mu) = \alpha(\mu - \lambda)B_{k+2,l}(\mu)D_{k+1,l-1}(\lambda) + \beta_{k+1}(\lambda - \mu)B_{k+2,l}(\lambda)D_{k+1,l-1}(\mu),$$
(18.32)

where

$$\alpha(\lambda) = \frac{h(\lambda - \eta)}{h(\lambda)}, \qquad \beta_l(\lambda) = \frac{h(\eta)h(\tau_{2l} - \lambda)}{h(-\lambda)h(\tau_{2l})}.$$
(18.33)

For the chain of N sites, we propose an infinite family of generating vectors

$$\Omega_N^l = \omega_1^l \otimes \omega_2^l \otimes \dots \otimes \omega_N^l, \tag{18.34}$$

where l is an arbitrary integer. In analogy with the six-vertex model, we want the gauge-transformed Lax operator (18.23) to possess the triangle form with the zero element

$$\gamma_n^l(\lambda)\omega_n^l = 0. \tag{18.35}$$

It is easy to check by using the addition theorems for the Jacobi theta functions that this condition is ensured by the choice

$$\omega_n^l = X_{n+l}(0). \tag{18.36}$$

The action of Lax-operator elements of interest α_n^l and β_n^l on the local vectors is simple, but non-diagonal,

$$\alpha_n^l(\lambda)\omega_n^l = h(\lambda + \eta)\omega_n^{l-1}, \qquad \delta_n^l(\lambda)\omega_n^l = h(\lambda)\omega_n^{l+1}.$$
(18.37)

Since $\mathcal{T}^{l}(\lambda) = \mathcal{T}_{N+l,l}$, we obtain from the local formulas (18.35)–(18.37) the following relations for the action of monodromy elements on the generating chain vectors: $C_{N+l,l}\Omega_{N}^{l} = 0$ and

$$A_{N+l,l}(\lambda)\Omega_n^l = h^N(\lambda+\eta)\Omega_n^{l-1}, \qquad D_{N+l,l}(\lambda)\Omega_n^l = h^N(\lambda)\Omega_n^{l+1}.$$
(18.38)

We are now ready to diagonalize the transfer matrix (18.28) by the generalized QISM technique. As the ansatz eigenvector we propose

$$\Psi_l(\lambda_1, \dots, \lambda_M) = \prod_{j=1}^M B_{l+j, l-j}(\lambda_j) \,\Omega_N^{l-M},\tag{18.39}$$

where M is an as-yet unspecified positive integer. Let us first investigate the action of the operator $A_{l,l}(\lambda)$ on this vector. Using successively the permutation relation (18.31) for $k = l, l+1, \ldots, l+M-1$, we commute $A_{l,l}(\lambda)$ with $B_{l+1,l-1}(\lambda_1)$, the consequent $A_{l+1,l-1}(\lambda)$ with $B_{l+2,l-2}(\lambda_1)$, etc., to end up with $A_{l+M,l-M}$ just ahead of the vector Ω_N^{l-M} . It follows from (18.38) that the operator $A_{l+M,l-M}$ can be applied to Ω_N^{l-M} only if M = N/2 (for simplicity, N is even). The result of the commutation procedure can be written as

$$A_{l,l}(\lambda)\Psi_l(\lambda_1,\ldots,\lambda_M) = {}_1t(\lambda;\lambda_1,\ldots,\lambda_M)\Psi_{l-1}(\lambda_1,\ldots,\lambda_M) + \sum_{j=1}^M {}_1t_j^l(\lambda;\lambda_1,\ldots,\lambda_M)\Psi_{l-1}(\lambda_1,\ldots,\lambda_{j-1},\lambda,\lambda_{j+1},\ldots,\lambda_M),$$
(18.40)

where

$${}_{1}t(\lambda;\lambda_{1},\ldots,\lambda_{M}) = h^{N}(\lambda+\eta)\prod_{j=1}^{M}\alpha(\lambda-\lambda_{j})$$
(18.41)

and

$${}_{1}t_{j}^{l}(\lambda;\lambda_{1},\ldots,\lambda_{M}) = -\beta_{l-1}(\lambda-\lambda_{j})h^{N}(\lambda_{j}+\eta)\prod_{\substack{k=1\\(k\neq j)}}^{M}\alpha(\lambda_{j}-\lambda_{k})$$
(18.42)

(j = 1, 2, ..., M). Here we assume that all λ_j are distinct. Proceeding similarly in the case of the operator $D_{l,l}(\lambda)$ applied to the ansatz vector (18.39), we obtain

$$D_{l,l}(\lambda)\Psi_l(\lambda_1,\ldots,\lambda_M) = {}_2t(\lambda;\lambda_1,\ldots,\lambda_M)\Psi_{l+1}(\lambda_1,\ldots,\lambda_M) + \sum_{j=1}^M {}_2t_j^l(\lambda;\lambda_1,\ldots,\lambda_M)\Psi_{l+1}(\lambda_1,\ldots,\lambda_{j-1},\lambda,\lambda_{j+1},\ldots,\lambda_M),$$
(18.43)

where

$${}_{2}t(\lambda;\lambda_{1},\ldots,\lambda_{M}) = h^{N}(\lambda) \prod_{j=1}^{M} \alpha(\lambda_{j} - \lambda)$$
(18.44)

and

$${}_{2}t_{j}^{l}(\lambda;\lambda_{1},\ldots,\lambda_{M}) = \beta_{l+1}(\lambda-\lambda_{j})h^{N}(\lambda_{j})\prod_{\substack{k=1\\(k\neq j)}}^{M}\alpha(\lambda_{k}-\lambda_{j})$$
(18.45)

 $(j=1,2,\ldots,M).$

We sum together Eqs. (18.40) and (18.43), multiply the addition by $\exp(2\pi i l\varphi)$, where $\varphi \in \langle 0, 1 \rangle$, and finally sum over all integers l from $-\infty$ to ∞ . The result is

$$T(\lambda)\Psi_{\varphi}(\lambda_{1},\ldots,\lambda_{M}) = t_{\varphi}(\lambda;\lambda_{1},\ldots,\lambda_{M})\Psi_{\varphi}(\lambda_{1},\ldots,\lambda_{M})$$
$$+ \sum_{l=-\infty}^{\infty} e^{2\pi i l\varphi} \sum_{j=1}^{M} t_{j,\varphi}^{l}(\lambda;\lambda_{1},\ldots,\lambda_{M})\Psi_{l}(\lambda_{1},\ldots,\lambda_{j-1},\lambda,\lambda_{j+1},\ldots,\lambda_{M}), \quad (18.46)$$

where

$$\Psi_{\varphi}(\lambda_1, \dots, \lambda_M) = \sum_{l=-\infty}^{\infty} e^{2\pi i l \varphi} \psi_l(\lambda_1, \dots, \lambda_M), \qquad (18.47)$$

$$t_{\varphi}(\lambda;\lambda_1,\ldots,\lambda_M) = e^{2\pi i\varphi} t(\lambda;\lambda_1,\ldots,\lambda_M) + e^{-2\pi i\varphi} t(\lambda;\lambda_1,\ldots,\lambda_M)$$
(18.48)

and

$$t_{j,\varphi}^{l}(\lambda;\lambda_{1},\ldots,\lambda_{M}) = e^{2\pi i\varphi} t_{j}^{l+1}(\lambda;\lambda_{1},\ldots,\lambda_{M}) + e^{-2\pi i\varphi} t_{j}^{l-1}(\lambda;\lambda_{1},\ldots,\lambda_{M}).$$
(18.49)

 $\Psi_{\varphi}(\lambda_1, \ldots, \lambda_M)$ is an eigenfunction of $T(\lambda)$ if the unwanted terms $t_{j,\varphi}^l(\lambda; \lambda_1, \ldots, \lambda_M)$ vanish. This requirement implies the Bethe ansatz equations for rapidities

$$\left[\frac{h(\lambda_j)}{h(\lambda_j+\eta)}\right]^N = e^{4\pi i\varphi} \prod_{\substack{k=1\\(k\neq j)}}^M \frac{h(\lambda_j-\lambda_k-\eta)}{h(\lambda_j-\lambda_k+\eta)}, \qquad j=1,\dots,M.$$
(18.50)

The corresponding eigenvalue is given by

$$t_{\varphi}(\lambda;\lambda_{1},\ldots,\lambda_{M}) = e^{2\pi i\varphi}h^{N}(\lambda+\eta)\prod_{j=1}^{M}\frac{h(\lambda_{j}-\lambda+\eta)}{h(\lambda_{j}-\lambda)} + e^{-2\pi i\varphi}h^{N}(\lambda)\prod_{j=1}^{M}\frac{h(\lambda-\lambda_{j}+\eta)}{h(\lambda-\lambda_{j})}.$$
(18.51)

Note that the eigenvalues are independent of the free parameters s and t.

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18.2 Restricted models and the φ parameter

The Bethe solution is not complete, two points are obscure at this stage. Firstly, for general values of η , we have the restriction M = N/2; we recall that for the six-vertex model M can take any integer value between 0 and N. In this part we shall show that for particular values of η the permissible values of M are less restricted. The second point concerns the introduction of a free parameter φ into the Bethe solution. The value of this angle parameter is obviously associated with the convergence of the series (18.47). It is expected that this series is summable to zero for all φ , except finitely many values φ_j . For these φ_j , our Bethe ansatz solution describes the eigenfunctions and eigenvalues of the transfer matrix. It turns out that the two problems are interwoven: The determination of the set $\{\varphi_j\}$ is relatively simple for η -values at which the permissible values of M are less restricted.

Let us first assume that there exists $Q \in \mathbb{Z}_{>0}$ such that

$$Q\eta = 4K. \tag{18.52}$$

Then H(u) and $\Theta(u)$ have the period $Q\eta$:

$$H(u + Q\eta) = H(u), \qquad \Theta(u + Q\eta) = \Theta(u). \tag{18.53}$$

The vector basis (18.2)–(18.6) has the periodicity $l \rightarrow l + Q$ which restricts the possible values of l to l = 0, 1, ..., Q - 1. The periodicity extends to the monodromy matrices $\mathcal{T}_{k,l}$ and to their operator entries which are periodic in k and l with period Q. The admissible values of M in the ansatz eigenvector (18.39) are now determined by the condition

$$2M = N \pmod{Q}.\tag{18.54}$$

If moreover N is a multiple of Q, then the admissible values of M are $0, Q, \ldots, N$ for odd Q and $0, Q/2, \ldots, N$ for even Q. The angle parameter of interest φ takes only the values

$$\varphi = \frac{m}{Q}, \qquad m = 0, 1, \dots, Q - 1.$$
 (18.55)

In sums of type (18.47) it is sufficient to sum over the period Q,

$$\Psi_{\varphi}(\lambda_1, \dots, \lambda_M) = \sum_{l=0}^{Q-1} e^{2\pi i lm/Q} \psi_l(\lambda_1, \dots, \lambda_M).$$
(18.56)

In a more general case

 $Q\eta = 4m_1 K \tag{18.57}$

with m_1 being an integer, for the given integer ν we define an integer m from the congruence

$$m = m_1 \nu \pmod{Q}. \tag{18.58}$$

Since φ may be shifted by an arbitrary integer, we can substitute φ in Eqs. (18.50) and (18.51) by $\nu \eta/(4K)$. Assuming the continuous dependence of the transfer matrix on η , this choice remains valid for all η for which the ratio η/K is real; M = N/2 for the unrestricted values of η .

We now assume that

$$Q\eta = 4m_1 K + i2m_2 K', (18.59)$$

where $Q \in \mathbb{Z}_{>0}$ and m_1 , m_2 are arbitrary nonzero integers. The Jacobi theta functions are quasi-doubly periodic with quasi-periods 2K and 2iK' (see Appendix B of paper I). The quasiperiodicity can be transformed to the periodicity by rescaling the Jacobi theta functions by a common prefactor. In particular, setting $A = i\pi m_2/(2KQ\eta)$ and defining the modified Jacobi theta functions

$$\tilde{H}(u) = e^{A(u-K)^2} H(u), \qquad \tilde{\Theta}(u) = e^{A(u-K)^2} \Theta(u), \qquad (18.60)$$

we have the periodicity relations

$$\tilde{H}(u+Q\eta) = \tilde{H}(u), \qquad \tilde{\Theta}(u+Q\eta) = \tilde{\Theta}(u)$$
(18.61)

analogous to those in Eq. (18.53). We introduce the scattering \tilde{S} -matrix with the texture of the S-matrix (18.1) and the elements

$$\widetilde{a}(\lambda) = \widetilde{\Theta}(-\eta)\widetilde{\Theta}(-\lambda)\widetilde{H}(\lambda+\eta),
\widetilde{b}(\lambda) = -\widetilde{\Theta}(-\eta)\widetilde{H}(-\lambda)\widetilde{\Theta}(\lambda+\eta),
\widetilde{c}(\lambda) = -\widetilde{H}(-\eta)\widetilde{\Theta}(-\lambda)\widetilde{\Theta}(\lambda+\eta),
\widetilde{d}(\lambda) = \widetilde{H}(-\eta)\widetilde{H}(-\lambda)\widetilde{H}(\lambda+\eta).$$
(18.62)

It can be checked that the elements of the \tilde{S} -matrix differ from the corresponding ones of the S-matrix only by the common prefactor $\exp\{A[2(\lambda^2 + \eta^2 + \lambda\eta) + 3K^2]\}$. The addition theorems (18.12) and (18.13) remain valid for the modified theta functions provided that g(u) is replaced by $\tilde{g}(u) = \tilde{\Theta}(-u)\tilde{H}(u)$. The monodromy matrices $\tilde{T}_{k,l}(\lambda)$, constructed from the elements (18.62) of the \tilde{S} -matrix, are periodic functions of k and l with the period Q. The algebra of the operators $\tilde{A}_{k,l}$, $\tilde{B}_{k,l}$, and $\tilde{D}_{k,l}$ is analogous to that described by the relations (18.30)–(18.33) provided that we replace h(u) by $\tilde{h}(u) = \tilde{\Theta}(0)\tilde{\Theta}(-u)\tilde{H}(u)$. As before, we propose the ansatz for eigenvectors of the transfer matrix $\tilde{T}(\lambda) = \tilde{A}_{l,l}(\lambda) + \tilde{D}_{l,l}(\lambda)$ in the form

$$\tilde{\Psi}_l(\lambda_1,\dots,\lambda_M) = \prod_{j=1}^M \tilde{B}_{l+j,l-j}(\lambda_j) \,\tilde{\Omega}_N^{l-M}.$$
(18.63)

By virtue of the periodicity in l we have the condition $2M = N \pmod{Q}$. Simultaneously, the angle parameter $\tilde{\varphi} = m/Q$ where $m = 0, 1, \dots, Q - 1$. The commutation procedure of the operators $\tilde{A}_{l,l}(\lambda)$ and $\tilde{D}_{l,l}(\lambda)$ with the sequence of \tilde{B} -operators in (18.63) leads to the eigenvalues of the transfer matrix $\tilde{T}(\lambda)$ of the form

$$\tilde{t}_{m}(\lambda;\lambda_{1},\ldots,\lambda_{M}) = e^{2\pi i m/Q} \tilde{h}^{N}(\lambda+\eta) \prod_{j=1}^{M} \frac{\tilde{h}(\lambda_{j}-\lambda+\eta)}{\tilde{h}(\lambda_{j}-\lambda)} + e^{-2\pi i m/Q} \tilde{h}^{N}(\lambda) \prod_{j=1}^{M} \frac{\tilde{h}(\lambda-\lambda_{j}+\eta)}{\tilde{h}(\lambda-\lambda_{j})}.$$
(18.64)

The rapidities $\{\lambda_j\}$ satisfy the system of Bethe equations

$$\left[\frac{\tilde{h}(\lambda_j)}{\tilde{h}(\lambda_j+\eta)}\right]^N = e^{4\pi i m/Q} \prod_{\substack{k=1\\(k\neq j)}}^M \frac{\tilde{h}(\lambda_j-\lambda_k-\eta)}{\tilde{h}(\lambda_j-\lambda_k+\eta)}, \qquad j=1,\dots,M.$$
(18.65)

We finally return from the modified to the ordinary Jacobi theta function via the transformation (18.60). The Bethe system of equations (18.65) becomes

$$\left[\frac{h(\lambda_j)}{h(\lambda_j+\eta)}\right]^N = e^{4\pi i\varphi(\lambda_j)} \prod_{\substack{k=1\\(k\neq j)}}^M \frac{h(\lambda_j-\lambda_k-\eta)}{h(\lambda_j-\lambda_k+\eta)}, \qquad j=1,\dots,M,$$
(18.66)

where the phase function $\varphi(\lambda)$ is defined by

$$\varphi(\lambda) = \frac{1}{Q} \left[m + \frac{m_2}{K} \sum_{k=1}^{M} \left(\lambda_k + \frac{\eta}{2} \right) + \frac{m_2}{2K} (N - 2M) \left(\lambda + \frac{\eta}{2} \right) \right].$$
(18.67)

The corresponding eigenvalues of the original transfer matrix $T(\lambda)$ are given by

$$t(\lambda;\lambda_1,\ldots,\lambda_M) = C \left[e^{2\pi i\varphi(\lambda)} h^N(\lambda+\eta) \prod_{j=1}^M \frac{h(\lambda_j-\lambda+\eta)}{h(\lambda_j-\lambda)} + e^{-2\pi i\varphi(\lambda)} h^N(\lambda) \prod_{j=1}^M \frac{h(\lambda-\lambda_j+\eta)}{h(\lambda-\lambda_j)} \right],$$
(18.68)

where $C = \exp[i\pi m_2\eta (N - 2M)/(2KQ)].$

18.3 XYZ chain: Bethe ansatz equations

The Hamiltonian of the XYZ Heisenberg model in zero magnetic field

$$H = -\frac{1}{2} \sum_{n=1}^{N} \left(J_x \boldsymbol{\sigma}_n^x \boldsymbol{\sigma}_{n+1}^x + J_y \boldsymbol{\sigma}_n^y \boldsymbol{\sigma}_{n+1}^y + J_z \boldsymbol{\sigma}_n^z \boldsymbol{\sigma}_{n+1}^z \right), \qquad \boldsymbol{\sigma}_{N+1}^{\alpha} \equiv \boldsymbol{\sigma}_1^{\alpha}$$
(18.69)

possesses useful symmetries. For an even number of sites N, using the unitary transformation

$$UHU^{-1}, \qquad U = \prod_{\text{even } n} \left(2\mathbf{S}_n^z \right) \tag{18.70}$$

we have the equivalence $H(J_x, J_y, J_z) \to H(-J_x, -J_y, J_z)$. Analogous equivalences are $H(J_x, J_y, J_z) \to H(J_x, -J_y, -J_z)$ and $H(J_x, J_y, J_z) \to H(-J_x, J_y, -J_z)$. This means that the Hamiltonian spectrum is unchanged under the sign reversal of two J_α 's; this was also the symmetry of the XXZ chain. Furthermore, the spectrum is invariant under exchanging J_α 's. It is therefore sufficient to study the case $0 \le |J_x| \le J_y \le J_z$.

The relationship between the transfer matrix of the eight-vertex model and the Hamiltonian of the XYZ Heisenberg chain was established in Sect. 8 of paper I. The coupling constants of the XYZ model were found to be parametrized as follows

$$J_x = 1 + k \operatorname{sn}^2 \eta, \qquad J_y = 1 - k \operatorname{sn}^2 \eta, \qquad J_z = \operatorname{cn} \eta \operatorname{dn} \eta,$$
 (18.71)

where the Jacobi elliptic functions have modulus k. The inverse relations for the parameters k and η read

$$k = \frac{1-l}{1+l}, \qquad l = \sqrt{\frac{J_z^2 - J_y^2}{J_z^2 - J_x^2}},$$
(18.72)

$$\mathrm{sn}^{2}\eta = -\frac{1}{k}\frac{J_{y} - J_{x}}{J_{y} + J_{x}} = -\left(\frac{\sqrt{J_{z}^{2} - J_{x}^{2}} + \sqrt{J_{z}^{2} - J_{y}^{2}}}{J_{y} + J_{x}}\right)^{2}.$$
(18.73)

Due to different normalizations of the S-matrix entries (8.13) and (18.1), the previous transfer matrix differs from the present one by the factor

$$\left[\frac{\mathrm{sn}(\lambda+\eta)}{\Theta(\eta)\Theta(\lambda)H(\lambda+\eta)}\right]^{N} = \left[\frac{1}{\sqrt{k}\Theta(\eta)}\right]^{N} \left[\frac{1}{\Theta(\lambda)\Theta(\lambda+\eta)}\right]^{N}.$$

This is why the present relationship between the XYZ Hamiltonian and the transfer matrix

$$H = -\operatorname{sn} \eta \frac{\mathrm{d}}{\mathrm{d}\lambda} \ln T(\lambda) \Big|_{\lambda=0} + N \left[\frac{J_z}{2} + \operatorname{sn} \eta \left(\frac{\Theta'(0)}{\Theta(0)} + \frac{\Theta'(\eta)}{\Theta(\eta)} \right) \right]$$
(18.74)

is slightly different from the previous one (8.24). From (18.68) we have

$$\frac{\mathrm{d}}{\mathrm{d}\lambda} \ln t(\lambda;\lambda_1,\ldots,\lambda_M)\Big|_{\lambda=0} = \frac{\mathrm{i}\pi m_2}{QK}(N-2M) + N\frac{h'(\eta)}{h(\eta)} \\ -\sum_{j=1}^M \left[\frac{h'(\lambda_j+\eta)}{h(\lambda_j+\eta)} - \frac{h'(\lambda_j)}{h(\lambda_j)}\right].$$
(18.75)

To symmetrize the obtained expressions in rapidities, in what follows we make the substitution $\lambda_j \rightarrow \lambda_j - \eta/2$. The Hamiltonian eigenvalues are thus expressible as

$$E(\lambda_1, \dots, \lambda_M) = \sum_{j=1}^M e(\lambda_j) - \operatorname{sn} \eta \, \frac{\mathrm{i}\pi m_2}{QK} (N - 2M) + N \left[\frac{\operatorname{cn} \eta \, \mathrm{dn} \, \eta}{2} + \operatorname{sn} \eta \left(\frac{\Theta'(\eta)}{\Theta(\eta)} - \frac{h'(\eta)}{h(\eta)} \right) \right],$$
(18.76)

where the energy component is given by

$$e(\lambda) = \operatorname{sn} \eta \left[\frac{h'\left(\lambda + \frac{\eta}{2}\right)}{h\left(\lambda + \frac{\eta}{2}\right)} - \frac{h'\left(\lambda - \frac{\eta}{2}\right)}{h\left(\lambda - \frac{\eta}{2}\right)} \right].$$
(18.77)

In terms of the shifted rapidities, the Bethe equations (18.66) take the form

$$\left[\frac{h\left(\lambda_{j}-\frac{\eta}{2}\right)}{h\left(\lambda_{j}+\frac{\eta}{2}\right)}\right]^{N} = e^{4\pi i\varphi(\lambda_{j})} \prod_{\substack{k=1\\(k\neq j)}}^{M} \frac{h(\lambda_{j}-\lambda_{k}-\eta)}{h(\lambda_{j}-\lambda_{k}+\eta)}, \qquad j=1,\ldots,M,$$
(18.78)

with

$$\varphi(\lambda) = \frac{1}{Q} \left[m + \frac{m_2}{K} \sum_{k=1}^M \lambda_k + \frac{m_2}{2K} (N - 2M) \lambda \right].$$
(18.79)

We would like to notice that, besides the XYZ Hamiltonian H with couplings (18.71), we can consider the "conjugate" XYZ Hamiltonian $\tilde{H} = -H$ with the couplings

$$J_x = -(1 + k \operatorname{sn}^2 \eta), \qquad J_y = -(1 - k \operatorname{sn}^2 \eta), \qquad J_z = -\operatorname{cn} \eta \operatorname{dn} \eta.$$
 (18.80)

The energy spectrum of \tilde{H} is related to that of H by reflection about the E = 0 axis. The relations (18.72) and (18.73) for the parameters k, η take the same form when expressed in terms of the couplings (18.80). The spectrum of \tilde{H} can be obtained following the same procedure as for H:

$$\tilde{E}(\lambda_1, \dots, \lambda_M) = \sum_{j=1}^M \tilde{e}(\lambda_j) + \operatorname{sn} \eta \, \frac{\mathrm{i}\pi m_2}{QK} (N - 2M) \\ -N \left[\frac{\operatorname{cn} \eta \, \mathrm{dn} \, \eta}{2} + \operatorname{sn} \eta \left(\frac{\Theta'(\eta)}{\Theta(\eta)} - \frac{h'(\eta)}{h(\eta)} \right) \right],$$
(18.81)

where the energy component is given by

$$\tilde{e}(\lambda) = \operatorname{sn} \eta \left[\frac{h'\left(\lambda - \frac{\eta}{2}\right)}{h\left(\lambda - \frac{\eta}{2}\right)} - \frac{h'\left(\lambda + \frac{\eta}{2}\right)}{h\left(\lambda + \frac{\eta}{2}\right)} \right]$$
(18.82)

and the rapidities λ_j are the solutions of the Bethe ansatz equations (18.78). The consideration of both H and \tilde{H} is important. If we find the eigenvector which corresponds to the largest eigenvalue of the transfer matrix, this eigenvector corresponds to either the ground state of Hand the state with the largest energy of \tilde{H} or vice versa.

18.4 XYZ chain: Ground state energy

In some basic domain of the parameters k and η , which will be specified later, the largest eigenvalue of the transfer matrix $T(\lambda)$ in the region close to $\lambda = 0$ is determined by the usual "antiferromagnetic" state. This state is characterized by m = 0 and M = N/2 rapidity solutions of the Bethe ansatz equations $\{\lambda_j\}$ which are real numbers, symmetrically distributed on the periodicity interval $\langle -K, K \rangle$, i.e.

$$-K \le \lambda_1 < \lambda_2 < \dots < \lambda_{N/2} \le K, \qquad \sum_{j=1}^{N/2} \lambda_j = 0.$$
 (18.83)

Under these conditions $\varphi(\lambda) = 0$ and the Bethe ansatz equations (18.78) take the simplified form

$$\left[\frac{h\left(\lambda_{j}-\frac{\eta}{2}\right)}{h\left(\lambda_{j}+\frac{\eta}{2}\right)}\right]^{N} = \prod_{\substack{k=1\\(k\neq j)}}^{N/2} \frac{h(\lambda_{j}-\lambda_{k}-\eta)}{h(\lambda_{j}-\lambda_{k}+\eta)}, \qquad j=1,\ldots,N/2.$$
(18.84)

The condition that the half-period K is real is equivalent to the requirement for the modulus $k \in (0, 1)$.

Taking the logarithm of (18.84) results in

$$N\theta(\lambda|\eta/2) = 2\pi I(\lambda) + \sum_{\lambda' \neq \lambda} \theta(\lambda - \lambda'|\eta), \qquad (18.85)$$

where $I(\lambda)$ is an increasing sequence of integers with unit step, localized in the interval -N/4 to N/4, and

$$\theta(\lambda|\eta) \equiv \frac{1}{i} \ln \frac{h(\lambda - \eta)}{h(\lambda + \eta)}.$$
(18.86)

Within the standard continualization procedure in the limit $N \to \infty$, we introduce the (absolute) ground state λ -density $\rho_0(\lambda)$, substitute $I(\lambda) = N \int_0^{\lambda} d\lambda' \rho(\lambda')$ and differentiate Eq. (18.85) with respect to λ , to obtain

$$G(\lambda|\eta/2) = \rho_0(\lambda) + \int_{-K}^{K} d\lambda' G(\lambda - \lambda'|\eta) \rho_0(\lambda'), \qquad (18.87)$$

where

$$G(\lambda|\eta) = \frac{1}{2\pi} \frac{\mathrm{d}}{\mathrm{d}\lambda} \theta(\lambda|\eta).$$
(18.88)

The kernel and the free term in Eq. (18.87) are periodic functions with period 2K. Since the integration is also over a period, we can solve this equation by using the discrete Fourier transform

$$f(\lambda) = \frac{1}{2K} \sum_{n=-\infty}^{\infty} e^{i\pi n\lambda/K} \hat{f}(n), \qquad \hat{f}(n) = \int_{-K}^{K} d\lambda \, e^{-i\pi n\lambda/K} f(\lambda), \tag{18.89}$$

namely

$$\hat{\rho}_0(n) = \frac{\hat{G}(n|\eta/2)}{1 + \hat{G}(n|\eta)}.$$
(18.90)

To find the Fourier transform of $G(\lambda|\eta)$, we first treat $\theta(\lambda|\eta)$ defined in (18.86) and express

$$\ln\frac{h(\lambda-\eta)}{h(\lambda+\eta)} = \ln\frac{\Theta(\lambda-\eta)H(\lambda-\eta)}{\Theta(\lambda+\eta)H(\lambda+\eta)} = \ln\frac{\vartheta_1\left(\frac{\lambda-\eta}{2K},q\right)}{\vartheta_1\left(\frac{\lambda+\eta}{2K},q\right)} + \ln\frac{\vartheta_4\left(\frac{\lambda-\eta}{2K},q\right)}{\vartheta_4\left(\frac{\lambda+\eta}{2K},q\right)}, \quad (18.91)$$

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where the real nome q of the theta functions is defined as $q = \exp(i\pi\tau) = \exp(-\pi K'/K) < 1$. From the infinite-product representation of ϑ_4 (B.22) we obtain

$$\ln \frac{\vartheta_4(u-v,q)}{\vartheta_4(u+v,q)} = -2\mathrm{i} \sum_{n=1}^{\infty} \frac{\sin(2\pi nu)\sin(2\pi nv)}{n\sin(\pi n\tau)},\tag{18.92}$$

where the principal branch of the logarithm was chosen. With the aid of the relation between ϑ_1 and ϑ_4 in (B.24), we have likewise

$$\ln \frac{\vartheta_1(u-v,q)}{\vartheta_1(u+v,q)} = i\pi + 2\pi i u - 2i \sum_{n=1}^{\infty} \frac{\sin(2\pi nu) \sin 2\pi n \left(v - \frac{\tau}{2}\right)}{n \sin(\pi n\tau)}.$$
(18.93)

Consequently,

$$\theta(\lambda|\eta) = \pi \left(1 + \frac{\lambda}{K}\right) + 2\sum_{n=1}^{\infty} \frac{\sin\left(\frac{\pi n\lambda}{K}\right)}{n\sinh\left(\frac{\pi nK'}{2K}\right)} \sinh\frac{\pi n}{2K} \left(2i\eta + K'\right).$$
(18.94)

This series is absolutely convergent provided that

$$|\operatorname{Im} \lambda| + |\operatorname{Im} \eta| < K', \qquad |\operatorname{Im} \lambda| + |\operatorname{Im} (\eta - \mathrm{i}K')| < K'.$$
(18.95)

For real λ , the real modulus k and the imaginary η are constrained to the principal domain

$$0 < k < 1, \qquad 0 \le -i\eta < K'.$$
 (18.96)

Eq. (18.88) tells us that the Fourier component $G(n|\eta) = 1$ for n = 0 and

$$\hat{G}(n|\eta) = \frac{\sinh\frac{\pi n}{2K}(2i\eta + K')}{\sinh\left(\frac{\pi nK'}{2K}\right)} \quad \text{for } n \neq 0.$$
(18.97)

With respect to (18.90), we finally arrive at

$$\hat{\rho}_0(n) = \frac{1}{2\cosh\left(\frac{\pi n i \eta}{2K}\right)}, \qquad \rho_0(\lambda) = \frac{1}{4K} \sum_{-\infty}^{\infty} \frac{\exp(i\pi n\lambda/K)}{\cosh\left(\frac{\pi n i \eta}{2K}\right)}.$$
(18.98)

For the parameters k and η in the principal domain (18.96), the following inequalities take place

$$|1 + k \operatorname{sn}^2 \eta| < 1 - k \operatorname{sn}^2 \eta < \operatorname{cn} \eta \operatorname{dn} \eta.$$
(18.99)

It can be shown by using perturbation theory [15] that the antiferromagnetic eigenvector corresponds to the ground state of the XYZ chain in the coupling region

$$|J_x| < -J_y < -J_z. (18.100)$$

We see that the corresponding Hamiltonian is \tilde{H} with the couplings (18.80). From (18.81) (taken with N = 2M) we have

$$\frac{\tilde{E}_0}{N} = 2\pi i \operatorname{sn} \eta \, \int_{-K}^{K} \mathrm{d}\lambda \, \rho_0(\lambda) G(\lambda|\eta/2) + \frac{J_z}{2} + \operatorname{sn}\eta \, \frac{H'(\eta)}{H(\eta)}.$$
(18.101)

Simple algebra gives

$$\frac{\tilde{E}_0}{N} = \frac{J_z}{2} + \frac{2\pi i}{K} \operatorname{sn} \eta \sum_{n=1}^{\infty} \frac{\sinh^2 \frac{\pi n}{2K} (i\eta + K')}{\sinh(\pi n K'/K)} \tanh\left(-\frac{\pi n}{2K} i\eta\right).$$
(18.102)

An equivalent form can be obtained by noticing that $(J_y - J_x)/2 = k \operatorname{sn}^2 \eta$ and [5]

$$k \operatorname{sn} \eta = -\frac{\pi \mathrm{i}}{K} \sum_{n=1}^{\infty} \left[\frac{\sinh\left(\frac{\pi n \mathrm{i} \eta}{2K}\right)}{\sinh\left(\frac{\pi n K'}{2K}\right)} - \frac{\sinh\left(\frac{\pi n \mathrm{i} \eta}{K}\right)}{\sinh\left(\frac{\pi n K'}{K}\right)} \right].$$
(18.103)

After some algebra, the ground-state energy (18.102) can be written as

$$\frac{E_0}{N} = \frac{1}{2}(J_z + J_y - J_x)
+ \frac{\pi i}{K} \operatorname{sn} \eta \sum_{n=1}^{\infty} \frac{\cosh\left[\frac{\pi n}{2K}(2i\eta + K')\right] - \cosh\left(\frac{\pi n}{2K}i\eta\right)}{\sinh\left(\frac{\pi nK'}{2K}\right)} \tanh\left(-\frac{\pi n}{2K}i\eta\right).(18.104)$$

18.5 XYZ chain: Critical ground-state properties

The ground state energy of the XYZ chain is an analytic function of the couplings J_x , J_y and J_z , except the case when two numerically largest couplings have equal magnitude. This fact was seen in the special case, the XXZ chain with $J_x = J_y = J$, when the system was in the critical state just for $\Delta = J_z/J$ from the interval (-1, 1). In the general case, the XYZ Hamiltonian (18.69) can be rewritten as

$$H(\Delta, \Gamma) \equiv \frac{2H}{J_x + J_y} = -\sum_{n=1}^{N} \left(\mathbf{S}_n^+ \mathbf{S}_{n+1}^- + \mathbf{S}_n^- \mathbf{S}_{n+1}^+ \right) + \Gamma \left(\mathbf{S}_n^+ \mathbf{S}_{n+1}^+ + \mathbf{S}_n^- \mathbf{S}_{n+1}^- \right) + \frac{\Delta}{2} \boldsymbol{\sigma}_n^z \boldsymbol{\sigma}_{n+1}^z,$$
(18.105)

where the dimensionless parameters

$$\Gamma = \frac{J_x - J_y}{J_x + J_y}, \qquad \Delta = \frac{2J_z}{J_x + J_y}$$
(18.106)

reflect the anisotropy in the (x, y) plane and along the z direction, respectively. The XXZ model corresponds to five constraints for parameters Γ and Δ : $\Delta = \pm(\Gamma + 1)$, $\Delta = \pm(\Gamma - 1)$ and $\Gamma = 0$. These lines are pictured in Fig. 18.1, the critical boundaries are depicted by heavy lines. The critical lines divide the (Δ, Γ) plane onto four sectors with different phases: z-ferromagnetic for $\Delta > 1$, z-antiferromagnetic for $\Delta < -1$, x-ferromagnetic for $\Gamma > 0$ and y-ferromagnetic for $\Gamma < 0$.

We now study the critical behavior of the ground state energy on the boundary $-J_y = -J_z$ of the principal region (18.100). As is seen from (18.72), this critical line corresponds to k = 1, k' = 0, i.e. $K \to \infty$, $K' = \pi/2$. To obtain the singular behavior of the ground state energy per site (18.104), we apply the Poisson summation formula

$$\sum_{n=-\infty}^{\infty} f(n\delta) = \frac{1}{\delta} \sum_{n=-\infty}^{\infty} \hat{f}(2\pi n/\delta), \qquad \hat{f}(k) = \int_{-\infty}^{\infty} \mathrm{d}x \,\mathrm{e}^{\mathrm{i}kx} f(x). \tag{18.107}$$



Fig. 18.1. Phase diagram of the XYZ model

Denoting

$$\mu = -\frac{\pi i \eta}{K'}, \qquad 0 < \mu < \pi, \tag{18.108}$$

and choosing $\delta = K'/(2K)$, the relation (18.104) can be rewritten as follows

$$\frac{\tilde{E}_0}{N} = \frac{1}{2}(J_z + J_y - J_x) + \frac{\pi i}{K'} \operatorname{sn} \eta \left[\hat{f}(0) + 2\sum_{n=1}^{\infty} \hat{f}\left(\frac{4\pi nK}{K'}\right) \right],$$
(18.109)

where

$$\hat{f}(k) = \int_{-\infty}^{\infty} \mathrm{d}x \, \exp(\mathrm{i}kx) \frac{\cosh(\pi - 2\mu)x - \cosh(\mu x)}{\sinh(\pi x)} \frac{\sinh(\mu x)}{\cosh(\mu x)}.$$
(18.110)

The summation over n in (18.109) can be performed in the integral representation of \hat{f} by using the formula

$$\sum_{n=1}^{\infty} \exp\left(\mathrm{i}k\frac{4\pi nK}{K'}\right) = \frac{p^{-2\mathrm{i}k}}{1 - p^{-2\mathrm{i}k}}, \qquad p = \exp(-2\pi K/K').$$
(18.111)

The integral in (18.110) can be closed by an infinite semi-circle in the complex upper half xplane. The poles inside the contour are x = im and $x = i\pi(m - \frac{1}{2})/\mu$ (m = 1, 2, ...). Using the residue theorem, we obtain

$$\frac{\tilde{E}_{0}}{N} = \frac{1}{2}(J_{z} + J_{y} - J_{x}) + \frac{\pi i}{K'} \operatorname{sn} \eta \left\{ \hat{f}(0) -4 \sum_{m=1}^{\infty} \left[\cos(2m\mu) \cos(m\pi) - \cos(m\mu) \right] \tan(m\mu) \frac{p^{2m}}{1 - p^{2m}} -\frac{4\pi}{\mu} \sum_{m=1}^{\infty} \cot \left[\left(m - \frac{1}{2} \right) \frac{\pi^{2}}{\mu} \right] \frac{p^{(2m-1)\pi/\mu}}{1 - p^{(2m-1)\pi/\mu}} \right\}.$$
(18.112)

The leading singular term is

$$\left(\tilde{E}_0/N\right)_{\rm sing} = -\frac{8\pi i}{\mu} \operatorname{sn} \eta \, \cot\left(\frac{\pi^2}{2\mu}\right) p^{\pi/\mu}.$$
(18.113)

Since

$$\operatorname{sn}(\eta, 1) = \frac{1}{\operatorname{i}} \frac{\operatorname{sn}(\operatorname{i}\eta, 0)}{\operatorname{cn}(\operatorname{i}\eta, 0)} = \operatorname{i} \operatorname{tan}\left(\frac{\mu}{2}\right), \quad J_y = -1 + \operatorname{sn}^2(\eta, 1) = -\frac{1}{\cos^2(\mu/2)}, \quad (18.114)$$

this expression simplifies to

$$\left(\tilde{E}_0/N\right)_{\rm sing} = \frac{4\pi\sin\mu}{\mu}(-J_y)\cot\left(\frac{\pi^2}{2\mu}\right)p^{\pi/\mu}.$$
 (18.115)

It can be easily shown that p behaves near the critical line like

$$p = \frac{1}{16} \frac{|J_z^2 - J_y^2|}{|J_z^2 - J_x^2|},$$
(18.116)

so that

$$\left(\tilde{E}_0/N\right)_{\text{sing}} \propto |J_z - J_y|^{\pi/\mu}, \qquad \cos\mu = \frac{J_x}{J_y}.$$
 (18.117)

We see that the critical index π/μ depends on model's parameters, which is in contradiction with universality hypothesis. Suzuki [48] however noticed that the ratio of arbitrary two critical indices is universal (weak universality).

19 Isotropic chain with arbitrary spin

The algebraic Bethe ansatz was used to establish higher-spin generalizations of the spin-1/2 Heisenberg models which are integrable. These generalizations cover a very restricted subspace of coupling constants between neighboring spins. The integrable spin-1 chains was considered in Ref. [53], the generalization to higher spin XXX chains was established by Kulish et al [49] who found an explicit form of the scattering matrix. The ground state and low-lying excitations were analyzed in [50]. The thermodynamics of the model was derived by Babujian [51,52]. The XXZ version of integrable higher-spin chains was introduced in [53] and solved in [54]. The higher-spin generalization of the XYZ spin chain was the subject of works [55,56]. For simplicity, here we consider only isotropic XXX chains.

19.1 Construction of the spin-s scattering matrix

In Sect. 7, we have constructed the isotropic scattering matrix acting in the space which is a tensor product of two-dimensional spin-1/2 Hilbert spaces defined at auxiliary sites ξ and η :

$$S_{\xi\eta}^{\frac{1}{2}\frac{1}{2}}(\lambda) = \mathcal{P}_{\xi\eta}^{\frac{1}{2}\frac{1}{2}} + \lambda I_{\xi\eta}^{\frac{1}{2}\frac{1}{2}} = \left(\lambda + \frac{1}{2}\right) I_{\xi\eta}^{\frac{1}{2}\frac{1}{2}} + \frac{1}{2} \left(\sigma_{\xi}, \sigma_{\eta}\right),$$
(19.1)

where the symbol $(A, B) = \sum_{\alpha=1}^{3} A^{\alpha} B^{\alpha}$ is used for the scalar product. It satisfies the YBE (7.18). The corresponding Lax operator, which couples an auxiliary site (say ξ) and site n = 1, 2, ..., N of the spin-1/2 chain, is given by

$$L_{\xi n}^{\frac{1}{2}\frac{1}{2}}(\lambda) = \left(\lambda + \frac{1}{2}\right) I_{\xi}^{\frac{1}{2}} \otimes I_{1...N}^{\frac{1}{2}\dots\frac{1}{2}} + \frac{1}{2} \left(\sigma_{\xi}, \boldsymbol{\sigma}_{n}\right).$$
(19.2)

The YBE for the scattering matrix can be transcribed in terms of Lax operators as follows

$$R_{\xi\eta}^{\frac{1}{2}\frac{1}{2}}(\lambda-\mu)\left[L_{\xin}^{\frac{1}{2}\frac{1}{2}}(\lambda)\otimes L_{\eta n}^{\frac{1}{2}\frac{1}{2}}(\mu)\right] = \left[L_{\xin}^{\frac{1}{2}\frac{1}{2}}(\mu)\otimes L_{\eta n}^{\frac{1}{2}\frac{1}{2}}(\lambda)\right]R_{\xi\eta}^{\frac{1}{2}\frac{1}{2}}(\lambda-\mu),$$
(19.3)

where

$$R_{\xi\eta}^{\frac{1}{2}\frac{1}{2}}(\lambda) = \mathcal{P}_{\xi\eta}^{\frac{1}{2}\frac{1}{2}}S_{\xi\eta}^{\frac{1}{2}\frac{1}{2}}(\lambda) = \left(1 + \frac{\lambda}{2}\right)I_{\xi\eta}^{\frac{1}{2}\frac{1}{2}} + \frac{\lambda}{2}\left(\sigma_{\xi}, \sigma_{\eta}\right).$$
(19.4)

The validity of Eq. (19.3) can be verified by applying the standard product relations for the Pauli matrices

$$(\sigma^{\alpha})^2 = I, \qquad \sigma^{\alpha} \sigma^{\beta} = i\epsilon_{\alpha\beta\gamma} \sigma^{\gamma}, \tag{19.5}$$

where $\epsilon_{\alpha\beta\gamma}$ is the antisymmetric tensor and the summation over repeated indices is considered.

Let us now have spin-s (s = 1/2, 1, 3/2, ...) variables instead of the spin-1/2 variables at each site n = 1, 2, ..., N of the chain. The local Hilbert space at each site has dimension 2s + 1. We define mixed Lax operators in the analogous way as before,

$$L_{\xi n}^{\frac{1}{2}s}(\lambda) = \left(\lambda + \frac{1}{2}\right) I_{\xi}^{\frac{1}{2}} \otimes I_{1...N}^{s...s} + (\sigma_{\xi}, \mathbf{S}_{n}).$$
(19.6)

It can be verified with the aid of (19.5) that the commutation relations between these Lax operators are intermediated by the spin-1/2 *R*-matrix (19.4),

$$R_{\xi\eta}^{\frac{1}{2}\frac{1}{2}}(\lambda-\mu)\left[L_{\xin}^{\frac{1}{2}s}(\lambda)\otimes L_{\eta n}^{\frac{1}{2}s}(\mu)\right] = \left[L_{\xin}^{\frac{1}{2}s}(\mu)\otimes L_{\eta n}^{\frac{1}{2}s}(\lambda)\right]R_{\xi\eta}^{\frac{1}{2}\frac{1}{2}}(\lambda-\mu).$$
(19.7)

The Lax-operator representation (19.6) is equivalent to the following expression for the S-matrix acting in the mixed spin-1/2 and spin-s Hilbert spaces:

$$S_{\xi\eta}^{\frac{1}{2}s}(\lambda) = \left(\lambda + \frac{1}{2}\right) I_{\xi}^{\frac{1}{2}} \otimes I_{\eta}^{s} + \left(\sigma_{\xi}, S_{\eta}\right).$$

$$(19.8)$$

Since the permutation operator is not defined for two spaces with distinct dimensions, the R-matrix is not defined for this case.

Assuming the spin-exchange symmetry between two sites, the formula (19.6) is equivalent to

$$L_{\xi n}^{s\frac{1}{2}}(\lambda) = \left(\lambda + \frac{1}{2}\right) I_{\xi}^{s} \otimes I_{1...N}^{\frac{1}{2}...\frac{1}{2}} + (S_{\xi}, \boldsymbol{\sigma}_{n}).$$
(19.9)

The analog of the commutation relation (19.7) is

$$R_{\xi\eta}^{ss}(\lambda-\mu) \left[L_{\xi\eta}^{s\frac{1}{2}}(\lambda) \otimes L_{\eta\eta}^{s\frac{1}{2}}(\mu) \right] = \left[L_{\xi\eta}^{s\frac{1}{2}}(\mu) \otimes L_{\eta\eta}^{s\frac{1}{2}}(\lambda) \right] R_{\xi\eta}^{ss}(\lambda-\mu).$$
(19.10)

Our next task is to solve this equation for the *R*-matrix acting in the tensor product of two spin-s Hilbert spaces. To simplify the notation, for a while we identify the auxiliary sites as $\xi \equiv 1$, $\eta \equiv 2$ and set $\sigma_n \equiv \sigma$. Thus the commutation relation (19.10) reads

$$R_{12}^{ss}(\lambda - \mu) \left[\lambda + \frac{1}{2} + (S_1, \sigma)\right] \left[\mu + \frac{1}{2} + (S_2, \sigma)\right]$$
$$= \left[\mu + \frac{1}{2} + (S_1, \sigma)\right] \left[\lambda + \frac{1}{2} + (S_2, \sigma)\right] R_{12}^{ss}(\lambda - \mu).$$
(19.11)

We shall look for the *R*-operator in the isotropic form $R_{12}^{ss}(\lambda, C)$ with a Casimir $C = (S_1, S_2)$. Since *R* is SL(2) invariant,

$$[R_{12}^{ss}(\lambda), S_1^{\alpha} + S_2^{\alpha}] = 0 \qquad \text{for all } \alpha = x, y, z, \tag{19.12}$$

Eq. (19.11) can be rewritten as follows

$$R_{12}^{ss}(\lambda) \left[\lambda(S_2, \sigma) + (S_1, \sigma)(S_2, \sigma)\right] = \left[\lambda(S_1, \sigma) + (S_1, \sigma)(S_2, \sigma)\right] R_{12}^{ss}(\lambda).$$
(19.13)

With regard to product relations of Pauli matrices (19.5), it holds

$$(S_1, \sigma)(S_2, \sigma) = (S_1, S_2) + i\epsilon_{\alpha\beta\gamma}\sigma^{\alpha}S_1^{\beta}S_2^{\gamma}.$$
(19.14)

Using this formula and the central property of Casimir operator, Eq. (19.13) can be transformed to

$$R_{12}^{ss}(\lambda) \left[\lambda S_2^{\alpha} + i\epsilon_{\alpha\beta\gamma} S_1^{\beta} S_2^{\gamma} \right] = \left[\lambda S_1^{\alpha} + i\epsilon_{\alpha\beta\gamma} S_1^{\beta} S_2^{\gamma} \right] R_{12}^{ss}(\lambda), \qquad \alpha = x, y, z.$$
(19.15)

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Due to the isotropic symmetry, it is sufficient to consider one from these three equations, say the combination

$$R_{12}^{ss}(\lambda) \left[\lambda S_2^+ + \left(S_2^z S_1^+ - S_1^z S_2^+\right)\right] = \left[\lambda S_1^+ + \left(S_2^z S_1^+ - S_1^z S_2^+\right)\right] R_{12}^{ss}(\lambda).$$
(19.16)

Instead of Casimir C, it is more convenient to look for the R-operator as a function of the operator J, introduced via

$$(S_1 + S_2)^2 = S_1^2 + S_2^2 + 2(S_1, S_2) = 2s(s+1) + 2(S_1, S_2) = J(J+1).$$
(19.17)

The operator J has an eigenvalue j in each irreducible representation D_j of the Clebsch-Gordan decomposition

$$D_s \otimes D_s = \sum_{j=0}^{2s} D_j.$$
 (19.18)

We shall solve Eq. (19.16) in the subspace of the highest vectors in each D_j , i.e.

$$S_1^+ + S_2^+ = 0, (19.19)$$

which is permissible due to the commutation relation

$$[S_1^+ S_2^z - S_1^z S_2^+, S_1^+ + S_2^+] = 0. (19.20)$$

With respect to the general formula

$$(S_1 + S_2)^2 = (S_1^z + S_2^z)^2 + S_1^z + S_2^z + (S_1^- + S_2^-)(S_1^+ + S_2^+),$$
(19.21)

we can identify

$$J = S_1^z + S_2^z \tag{19.22}$$

in the constrained subspace (19.19). Eq. (19.16) thus reduces to

$$R_{12}^{ss}(\lambda,J)\left(-\lambda S_1^+ + JS_1^+\right) = \left(\lambda S_1^+ + JS_1^+\right)R_{12}^{ss}(\lambda,J).$$
(19.23)

Using in this equation the commutation relation

$$S_1^+J = S_1^+(S_1^z + S_2^z) = (S_1^z + S_2^z - 1)S_1^+ = (J-1)S_1^+,$$
(19.24)

we obtain the functional equation

$$R_{12}^{ss}(\lambda, J)(-\lambda + J) = (\lambda + J)R_{12}^{ss}(\lambda, J - 1).$$
(19.25)

We search the R-operator in the form

$$R_{12}^{ss}(\lambda) = \sum_{j=0}^{2s} \rho_j(\lambda) P_{12}^j,$$
(19.26)

where P^j is a projector in the tensor product of two spin-s Hilbert spaces which fixes the state with total spin j, i.e. if $|l\rangle$ is a state with total spin l, then

$$P^{j}|l\rangle = \delta_{jl}|j\rangle. \tag{19.27}$$

It is clear from (19.17) that P_{12}^j can be represented as the polynomial of degree 2s in $x = (S_1, S_2)$,

$$P_{12}^{j} = \prod_{\substack{l=0\\l\neq j}}^{2s} \frac{x - x_{l}}{x_{j} - x_{l}}, \qquad x_{l} = \frac{1}{2} \left[l(l+1) - 2s(s+1) \right].$$
(19.28)

Within the representation (19.26), the functional equation (19.25) implies the recurrence relations

$$\rho_j(\lambda) = \frac{j+\lambda}{j-\lambda}\rho_{j-1}(\lambda) \tag{19.29}$$

which determine the coefficients $\rho_j(\lambda)$ up to a common prefactor. We choose

$$\rho_0(\lambda) = 1, \qquad \rho_j(\lambda) = \prod_{k=1}^j \frac{k+\lambda}{k-\lambda} \qquad j = 1, 2, \dots, 2s,$$
(19.30)

so that

$$R_{12}^{ss}(\lambda) = \sum_{j=0}^{2s} \prod_{k=1}^{j} \left(\frac{k+\lambda}{k-\lambda}\right) P_{12}^{j} = \sum_{j=0}^{2s} \prod_{k=1}^{j} \left(\frac{k+\lambda}{k-\lambda}\right) \prod_{\substack{l=0\\l\neq j}}^{2s} \frac{(S_1, S_2) - x_l}{x_j - x_l}.$$
 (19.31)

The normalization implies correctly the initial condition $R_{12}^{ss}(0) = \sum_{j=0}^{2s} P_{12}^j = I$. To obtain the S-matrix, we write down the Clebsch-Gordan decomposition

$$|s, m_1\rangle|s, m_2\rangle = \sum_{j=0}^{2s} \langle j, m_1 + m_2|s, m_1, s, m_2\rangle|j, m_1 + m_2, s, s\rangle.$$
(19.32)

The Clebsch-Gordan coefficients possess the symmetry

$$\langle j, m_1 + m_2 | s, m_1, s, m_2 \rangle = (-1)^{2s+j} \langle j, m_1 + m_2 | s, m_2, s, m_1 \rangle.$$
 (19.33)

Thus the permutation operator between two spin-s spaces, defined by $\mathcal{P}_{12}^{ss}|s,m_1\rangle|s,m_2\rangle = |s,m_2\rangle|s,m_1\rangle$, reads explicitly

$$\mathcal{P}_{12}^{ss} = (-1)^{2s} \sum_{j=0}^{2s} (-1)^j P_{12}^j. \tag{19.34}$$

Taking into account that $P^{j}P^{l} = \delta_{jl}P^{j}$, the S-matrix has the form

$$S_{12}^{ss}(\lambda) = \mathcal{P}_{12}^{ss} R_{12}^{ss}(\lambda) = (-1)^{2s} \sum_{j=0}^{2s} \prod_{k=1}^{j} \left(\frac{\lambda+k}{\lambda-k}\right) \prod_{\substack{l=0\\l\neq j}}^{2s} \frac{(S_1, S_2) - x_l}{x_j - x_l} \dots$$
(19.35)

The corresponding Lax operator acting on s-spins at the auxiliary site ξ and the chain site n,

$$L_{\xi n}^{ss}(\lambda) = (-1)^{2s} \sum_{j=0}^{2s} \prod_{k=1}^{j} \left(\frac{\lambda+k}{\lambda-k}\right) P_{\xi n}^{j},$$
(19.36)

satisfies the commutation relation

$$R_{\xi\eta}^{ss}(\lambda-\mu)\left[L_{\xi\eta}^{ss}(\lambda)\otimes L_{\eta\eta}^{ss}(\mu)\right] = \left[L_{\xi\eta}^{ss}(\mu)\otimes L_{\eta\eta}^{ss}(\lambda)\right]R_{\xi\eta}^{ss}(\lambda-\mu).$$
(19.37)

19.2 Algebraic Bethe ansatz

From now, each site n = 1, 2, ..., N of the chain is occupied by the spin-s, the spins localized at the auxiliary sites ξ and η may be either s or 1/2.

Our aim is to diagonalize the transfer matrix

$$T^{s}(\lambda) = \operatorname{Tr}_{\xi} \mathcal{T}^{s}_{\xi}(\lambda), \qquad \mathcal{T}^{s}_{\xi}(\lambda) = L^{ss}_{\xi 1}(\lambda) L^{ss}_{\xi 2}(\lambda) \cdots L^{ss}_{\xi N}(\lambda).$$
(19.38)

The YB commutation relation for Lax operators (19.37) implies an analogous relation for monodromy matrices

$$R_{\xi\eta}^{ss}(\lambda-\mu)\left[\mathcal{T}_{\xi}^{s}(\lambda)\otimes\mathcal{T}_{\eta}^{s}(\mu)\right] = \left[\mathcal{T}_{\xi}^{s}(\mu)\otimes\mathcal{T}_{\eta}^{s}(\lambda)\right]R_{\xi\eta}^{ss}(\lambda-\mu)$$
(19.39)

and an infinite family of commuting transfer matrices arises:

$$[T^{s}(\lambda), T^{s}(\mu)] = 0 \qquad \text{for arbitrary } \lambda \text{ and } \mu.$$
(19.40)

The eigenfunctions of $T^s(\lambda)$ do not depend on the spectral parameter λ . The logarithmic derivative of the transfer matrix $T^s(\lambda)$ with respect to λ , taken at $\lambda = 0$, leads to the spin-s Hamiltonian

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\ln T^{s}(\lambda)\Big|_{\lambda=0} = H^{s}, \qquad H^{s} = \sum_{n=1}^{N} H^{s}_{n,n+1}, \tag{19.41}$$

where the nearest neighbor interaction is given by

$$H_{n,n+1}^{s} = \frac{\mathrm{d}}{\mathrm{d}\lambda} R_{n,n+1}^{ss}(\lambda) \Big|_{\lambda=0} = \sum_{j=1}^{2s} \left(\sum_{k=1}^{j} \frac{2}{k} \right) \prod_{\substack{l=0\\l\neq j}}^{2s} \frac{(\mathbf{S}_{n}, \mathbf{S}_{n+1}) - x_{l}}{x_{j} - x_{l}}$$
(19.42)

with $H_{N,N+1} \equiv H_{N,1}$. Note that in the generic formula (8.21), the nearest-neighbor component of the Hamiltonian corresponds to the λ -derivative of the permuted S-matrix elements, i.e. of the R-matrix elements.

Although the $T^s(\lambda)$ matrices form the infinite commuting family, it is difficult to diagonalize them directly by using the algebraic Bethe ansatz. This is why we introduce auxiliary transfer matrices $T^{\frac{1}{2}}(\lambda)$ with spin-1/2 at the auxiliary site ξ , keeping spin-s at each chain site:

$$T^{\frac{1}{2}}(\lambda) = \operatorname{Tr}_{\xi} \mathcal{T}_{\xi}^{\frac{1}{2}}(\lambda), \qquad \mathcal{T}_{\xi}^{\frac{1}{2}}(\lambda) = L_{\xi 1}^{\frac{1}{2}s}(\lambda) L_{\xi 2}^{\frac{1}{2}s}(\lambda) \cdots L_{\xi N}^{\frac{1}{2}s}(\lambda).$$
(19.43)

The YB commutation relation for Lax operators (19.7) leads to

$$R_{\xi\eta}^{\frac{1}{2}\frac{1}{2}}(\lambda-\mu)\left[\mathcal{T}_{\xi}^{\frac{1}{2}}(\lambda)\otimes\mathcal{T}_{\eta}^{\frac{1}{2}}(\mu)\right] = \left[\mathcal{T}_{\xi}^{\frac{1}{2}}(\mu)\otimes\mathcal{T}_{\eta}^{\frac{1}{2}}(\lambda)\right]R_{\xi\eta}^{\frac{1}{2}\frac{1}{2}}(\lambda-\mu),$$
(19.44)

which implies an infinite family of commuting transfer matrices

$$[T^{\frac{1}{2}}(\lambda), T^{\frac{1}{2}}(\mu)] = 0 \qquad \text{for arbitrary } \lambda \text{ and } \mu. \tag{19.45}$$

To establish a relationship between the sets of commuting transfer matrices $T^s(\lambda)$ and $T^{\frac{1}{2}}(\lambda)$, we consider the "mixed" S-matrix (19.8). This S-matrix is an intertwiner for the commutation of the local Lax operators

$$S_{\xi\eta}^{\frac{1}{2}s}(\lambda-\mu)L_{\xin}^{\frac{1}{2}s}(\lambda)L_{\eta n}^{ss}(\mu) = L_{\eta n}^{ss}(\mu)L_{\xi n}^{\frac{1}{2}s}(\lambda)S_{\xi\eta}^{\frac{1}{2}s}(\lambda-\mu)$$
(19.46)

and, consequently, of the monodromy matrices

$$S_{\xi\eta}^{\frac{1}{2}s}(\lambda-\mu)\mathcal{T}_{\xi}^{\frac{1}{2}}(\lambda)\mathcal{T}_{\eta}^{s}(\mu) = \mathcal{T}_{\eta}^{s}(\mu)\mathcal{T}_{\xi}^{\frac{1}{2}}(\lambda)S_{\xi\eta}^{\frac{1}{2}s}(\lambda-\mu).$$
(19.47)

The non-existence of the mixed *R*-matrix is not a problem. We multiply directly Eq. (19.47) from left by the inverse matrix $[S_{\xi\eta}^{\frac{1}{2}s}(\lambda-\mu)]^{-1}$ and take the trace, with the result

$$[T^{\frac{1}{2}}(\lambda), T^{s}(\mu)] = 0 \qquad \text{for arbitrary } \lambda \text{ and } \mu.$$
(19.48)

This means that also the families $\{T^{\frac{1}{2}}(\lambda)\}$ and $\{T^{s}(\lambda)\}$ have common eigenvectors, independent of λ .

It is easy to diagonalize $T^{\frac{1}{2}}(\lambda)$ by using the procedure explained in Sect. 8.3. The spin-1/2 R-matrix (19.4) has the standard form (7.58) with the elements

$$a(\lambda) = 1 + \lambda, \quad b(\lambda) = \lambda, \quad c(\lambda) = 1, \quad d(\lambda) = 0.$$
 (19.49)

The monodromy matrix $T_{\xi}^{\frac{1}{2}}(\lambda)$ is expressible formally in the auxiliary $2 \times 2 \xi$ -space as follows

$$\mathcal{T}^{\frac{1}{2}}(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix}.$$
(19.50)

The relation (19.44) then implies exactly the same commutation formulas (8.34)–(8.36) for the operators $\{A, B, C, D\}$ as in the trigonometric spin-1/2 case. The Lax operator at site n with spin s has in the auxiliary ξ space the following form

$$L_n^s(\lambda) = \begin{pmatrix} \lambda + \frac{1}{2} + \mathbf{S}_n^z & \mathbf{S}_n^-\\ \mathbf{S}_n^+ & \lambda + \frac{1}{2} - \mathbf{S}_n^z \end{pmatrix}.$$
(19.51)

As the generating vector of the $(2s + 1)^N$ -dimensional Hilbert space, we take the direct product of the highest eigenvectors of S^z on the chain of N sites:

$$\Omega^{s} = \underbrace{e^{s}}_{1} \otimes \underbrace{e^{s}}_{2} \otimes \cdots \otimes \underbrace{e^{s}}_{N}, \qquad e^{s} = \begin{pmatrix} 1\\0\\\vdots\\0 \end{pmatrix} \begin{pmatrix} 1\\2\\\vdots\\2s+1 \end{pmatrix}$$
(19.52)

The Lax operator (19.51) is the identity operator at each site, except the *n*th site where it acts on e_n^s as follows

$$L_n^s(\lambda)e_n^s = \begin{pmatrix} \lambda + \frac{1}{2} + s & [\cdots] \\ 0 & \lambda + \frac{1}{2} - s \end{pmatrix} e_n^+.$$
(19.53)

Due to the triangle form of this matrix, the diagonal elements of the monodromy matrix $\mathcal{T}^{\frac{1}{2}}(\lambda)$ (19.50) act on the vector Ω^s as follows

$$A(\lambda)\Omega^{s} = \left(\lambda + \frac{1}{2} + s\right)^{N}\Omega^{s}, \qquad D(\lambda)\Omega^{s} = \left(\lambda + \frac{1}{2} - s\right)^{N}\Omega^{s}; \tag{19.54}$$

the action of B on Ω^s is given indirectly via its commutation relations with A (8.35) and D (8.36). The eigenvectors of the transfer matrix $T^{\frac{1}{2}}(\lambda) = A(\lambda) + D(\lambda)$ are searched in the ansatz form

$$\psi(\lambda_1, \dots, \lambda_M) = \prod_{\alpha=1}^M B(\lambda_\alpha) \Omega^s.$$
(19.55)

As before, the "unwanted" terms which arise from the commutation of operators B with A and D, namely

$$t_{\alpha}(\lambda;\lambda_{1},\ldots,\lambda_{M}) = -\frac{c(\lambda_{\alpha}-\lambda)}{b(\lambda_{\alpha}-\lambda)} \left[\left(\lambda_{\alpha}+\frac{1}{2}+s\right)^{N} \prod_{\substack{\beta=1\\(\beta\neq\alpha)}}^{M} \frac{a(\lambda_{\beta}-\lambda_{\alpha})}{b(\lambda_{\beta}-\lambda_{\alpha})} - \left(\lambda_{\alpha}+\frac{1}{2}-s\right)^{N} \prod_{\substack{\beta=1\\(\beta\neq\alpha)}}^{M} \frac{a(\lambda_{\alpha}-\lambda_{\beta})}{b(\lambda_{\alpha}-\lambda_{\beta})} \right]$$
(19.56)

 $(\alpha=1,2,\ldots,M),$ must vanish. These conditions imply the system of M nonlinear Bethe equations

$$\left(\frac{\lambda_{\alpha} + \frac{1}{2} + s}{\lambda_{\alpha} + \frac{1}{2} - s}\right)^{N} = \prod_{\substack{\beta=1\\(\beta\neq\alpha)}}^{M} \left(\frac{\lambda_{\alpha} - \lambda_{\beta} + 1}{\lambda_{\alpha} - \lambda_{\beta} - 1}\right) \qquad \alpha = 1, 2, \dots, M,$$
(19.57)

which determines the rapidity parameters $\{\lambda_1, \lambda_2, \dots, \lambda_M\}$. We note that the total spin zprojection $\mathbf{S}^z = \sum_{n=1}^{N} \mathbf{S}_n^z$, when acting on the Bethe vector (19.55), has eigenvalues Ns - M, so M can take the values $0, 1, \dots, 2Ns$. With respect to the $\mathbf{S}^z \to -\mathbf{S}^z$ symmetry, it is sufficient to consider $M = 0, 1, \dots, Ns$ (if Ns is integer).

We are now ready to diagonalize the transfer matrix $T^{s}(\lambda)$, which is the trace of the monodromy matrix \mathcal{T}^{s} ,

$$T^{s}(\lambda) = \sum_{m=-s}^{s} \mathcal{T}^{s}_{m,m}(\lambda).$$
(19.58)

We know that the eigenvectors of $T^s(\lambda)$ are given by (19.55), where $\{\lambda_1, \ldots, \lambda_M\}$ satisfy the Bethe equations (19.57). To find the eigenvalues of $T^s(\lambda)$, we have to derive the commutation relations between the monodromy diagonal elements $\mathcal{T}^s_{m,m}(\lambda)$ and the operator $B(\mu)$ as well as their action on the generating vector Ω^s .

The commutation relations follow from Eq. (19.47):

$$\mathcal{T}_{m,m}^{s}(\lambda)B(\mu) = \beta_{m}^{s}(\mu - \lambda)B(\mu)\mathcal{T}_{m,m}^{s}(\lambda) + \text{ unwanted terms,}$$
(19.59)

where

$$\beta_m^s(\lambda) = \frac{\left(\lambda - \frac{1}{2} - s\right)\left(\lambda + \frac{1}{2} + s\right)}{\left(\lambda - \frac{1}{2} - m\right)\left(\lambda + \frac{1}{2} - m\right)}$$
(19.60)

and the unwanted terms disappear due to (19.57).

To accomplish the second task, using the Clebsch-Gordan decomposition (19.32) we first act by matrix elements of the Lax-operator (19.36) in the auxiliary ξ -space on the generating vector $e^s = |s, s\rangle$ at site *n*, to obtain

$$\langle s, m' | L^{ss}_{\xi n}(\lambda) | s, m \rangle | s, s \rangle = (-1)^{2s} \sum_{j=0}^{2s} \prod_{k=1}^{j} \left(\frac{\lambda+k}{\lambda-k} \right) \langle j, m+s | s, m, s, s \rangle$$

$$\times \langle s, m' | j, m+s, s, s \rangle.$$

$$(19.61)$$

Using the Clebsch-Gordan decomposition inverse to (19.32), we have

$$\langle s, m' | j, m + s, s, s \rangle = \langle s, m', s, m_2 | j, m + s \rangle | s, m_2 \rangle, \qquad m_2 = m + s - m'.$$
 (19.62)

Since $m_2 \leq s$, we find that

$$\langle s, m' | L^{ss}_{\xi n}(\lambda) | s, m \rangle | s, s \rangle = 0 \qquad \text{for } m' < m, \tag{19.63}$$

i.e. the local Lax-operator has the triangle form in the auxiliary ξ -space, as was expected. The vector $|s, s\rangle$ is the eigenvector for the diagonal m' = m elements of the monodromy matrix

$$\langle s, m | L^{ss}_{\xi n}(\lambda) | s, m \rangle | s, s \rangle = \alpha^s_m(\lambda) | s, s \rangle, \qquad m = -s, -s + 1, \dots, s$$
(19.64)

with the eigenvalues

$$\alpha_m^s(\lambda) = (-1)^{2s} \sum_{j=0}^{2s} \prod_{k=1}^j \left(\frac{\lambda+k}{\lambda-k}\right) \langle j, m+s|s, m, s, s\rangle^2.$$
(19.65)

Explicitly, we have

$$\alpha_s^s(\lambda) = \prod_{k=1}^{2s} \left(\frac{k+\lambda}{k-\lambda}\right), \qquad \alpha_m^s(\lambda) = \alpha_s^s(\lambda) \prod_{l=m+1}^s \left(\frac{\lambda+l-s}{\lambda+l+s}\right) \quad \text{for } m < s.$$
(19.66)

Since the monodromy matrix is the product of N local Lax-operators of triangle form, it holds

$$\mathcal{T}^s_{m,m}(\lambda)\Omega^s = \left[\alpha^s_m(\lambda)\right]^N \Omega^s \qquad m = -s, -s+1, \dots, s.$$
(19.67)

Taking into account the commutation relations (19.59), we conclude that the eigenvalue of the transfer matrix $T^s(\lambda)$ corresponding to the eigenvector (19.55) is given by

$$t^{s}(\lambda;\lambda_{1},\ldots,\lambda_{M}) = \sum_{m=-s}^{s} \left[\alpha_{m}^{s}(\lambda)\right]^{N} \prod_{\alpha=1}^{M} \beta_{m}^{s}(\lambda_{\alpha}-\lambda).$$
(19.68)

Since $\alpha_m^s(\lambda) \propto \lambda$ for m < s, only the m = s term contributes to the logarithmic derivative of t^s at $\lambda = 0$. The eigenvalues of the Hamiltonian H^s (19.41), (19.42) thus read

$$E^{s}(\lambda_{1},\ldots,\lambda_{M}) = \frac{\partial \ln t^{s}}{\partial \lambda}\Big|_{\lambda=0} = N \sum_{k=1}^{2s} \frac{2}{k} + \sum_{\alpha=1}^{M} \frac{2s}{\left(\lambda_{\alpha} + \frac{1}{2}\right)^{2} - s^{2}}.$$
(19.69)

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It is convenient to subtract the absolute term from the Hamiltonian, i.e. $H^s = \sum_{n=1}^{N} H^s_{n,n+1}$ with

$$H_{n,n+1}^{s} = \sum_{j=1}^{2s} \left(\sum_{k=1}^{j} \frac{2}{k} \right) \prod_{\substack{l=0\\l\neq j}}^{2s} \frac{(\mathbf{S}_{n}, \mathbf{S}_{n+1}) - x_{l}}{x_{j} - x_{l}} - \sum_{k=1}^{2s} \frac{2}{k}.$$
(19.70)

This ensures that $H_{n,n+1}^s |s,s\rangle \otimes |s,s\rangle = 0$. The integrable spin-s Hamiltonians are antiferromagnetic. For the case s = 1/2, we have

$$H_{n,n+1}^{\frac{1}{2}} = 2\left(\mathbf{S}_n \cdot \mathbf{S}_{n+1} - \frac{1}{4}\right) = \frac{1}{2}\left(\boldsymbol{\sigma}_n \cdot \boldsymbol{\sigma}_{n+1} - 1\right).$$
(19.71)

For the case s = 1, we have

$$H_{n,n+1}^{1} = \frac{1}{2} \left[\mathbf{S}_{n} \cdot \mathbf{S}_{n+1} - \left(\mathbf{S}_{n} \cdot \mathbf{S}_{n+1} \right)^{2} \right],$$
(19.72)

etc. After rescaling and shifting $\lambda_{\alpha} \rightarrow i\lambda_{\alpha} - 1/2$, the energy (19.69) (with the absolute term subtracted) takes the form

$$E^{s}(\lambda_{1},...,\lambda_{M}) = -\sum_{\alpha=1}^{M} \frac{2s}{\lambda_{\alpha}^{2} + s^{2}}$$
(19.73)

and the Bethe equations (19.57) become

$$\left(\frac{\lambda_{\alpha} - is}{\lambda_{\alpha} + is}\right)^{N} = \prod_{\substack{\beta=1\\(\beta \neq \alpha)}}^{M} \left(\frac{\lambda_{\alpha} - \lambda_{\beta} - i}{\lambda_{\alpha} - \lambda_{\beta} + i}\right) \qquad \alpha = 1, 2, \dots, M.$$
(19.74)

19.3 Thermodynamics with strings

As $N \to \infty$, the solutions of the Bethe equations (19.74) are strings of lengths n = 1, 2, ...,

$$\lambda_{\alpha}^{(n,r)} = \lambda_{\alpha}^{n} + i\left(\frac{n+1}{2} - r\right), \qquad r = 1, 2, \dots, n,$$
(19.75)

where the centers λ_{α}^{n} ($\alpha = 1, ..., M_{n}$) lie on the real axis. The numbers M_{n} of *n*-strings are constrained by $\sum_{n=1}^{\infty} nM_{n} = M$. The Bethe equations (19.74) can be expressed in terms of the string centers as follows

$$N\theta_{n,2s}(\lambda_{\alpha}^{n}) = 2\pi I_{\alpha}^{n} + \sum_{m=1}^{\infty} \sum_{\beta=1}^{M_{m}} \Theta_{nm}(\lambda_{\alpha}^{n} - \lambda_{\beta}^{m}),$$
(19.76)

where I_{α}^{n} are integers or half-integers,

$$\theta_{nm}(\lambda) = \sum_{r=1}^{n} \theta_m\left(\lambda^{(n,r)}\right) = \sum_{l=1}^{\min(n,m)} \theta_{n+m+1-2l}(\lambda)$$
(19.77)

with $\theta_n(\lambda) \equiv 2 \arctan(2\lambda/n)$ and $\Theta_{nm}(\lambda)$ is defined in (16.14). The energy (19.73) of a given collection of strings is written as

$$E^{s}(\lambda_{1},\ldots,\lambda_{M}) = \sum_{n=1}^{\infty} \sum_{\alpha=1}^{M_{n}} E^{s}_{n}(\lambda_{\alpha}^{n}), \qquad (19.78)$$

where

$$E_n^s(\lambda) = -\sum_{r=1}^n \frac{2s}{\left(\lambda^{(n,r)}\right)^2 + s^2} = -\frac{\mathrm{d}}{\mathrm{d}\lambda} \theta_{n,2s}(\lambda).$$
(19.79)

To derive the thermodynamics of the integrable spin-s chains, we proceed in close analogy with the isotropic spin-1/2 antiferromagnetic (J = -1) chain in Sect. 16.1. The distributions of the real *n*-string particle centers $\rho_n(\lambda)$ and hole centers $\tilde{\rho}_n(\lambda)$ are constrained by

$$\tilde{\rho}_n + \sum_{m=1}^{\infty} A_{nm} * \rho_m = a_n \qquad (n = 1, 2, ...),$$
(19.80)

where the Fourier transform of the matrix $A_{nm}(\lambda)$ is presented in Eq. (16.28) and a_n is given by

$$a_n(\lambda) = \frac{1}{2\pi} \frac{\mathrm{d}\theta_{n,2s}(\lambda)}{\mathrm{d}\lambda}, \qquad \hat{a}_n(\omega) = \hat{s}(\omega)\hat{A}_{n,2s}(\omega).$$
(19.81)

The total energy per site from all strings is given by

$$\frac{E}{N} = -2sh + \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} d\lambda \left[-2\pi a_n(\lambda) + 2nh \right] \rho_n(\lambda).$$
(19.82)

The equilibrium state is determined by the variational condition for the free energy $\delta F = \delta E - T\delta S = 0$. Using the relations

$$\sum_{n=1}^{\infty} \left(A_{n'n}^{-1} \star a_n \right) (\lambda) = s(\lambda) \delta_{n',2s}, \qquad \sum_{n=1}^{\infty} A_{n'n}^{-1} \star n = 0, \tag{19.83}$$

the variational condition leads to an infinite sequence of the TBA equations for the ratios $\eta_n(\lambda) = \tilde{\rho}_n^{eq}(\lambda)/\rho_n^{eq}(\lambda)$:

$$\ln \eta_n(\lambda) = -\frac{2\pi}{T} s(\lambda) \delta_{n,2s} + \int_{-\infty}^{\infty} d\lambda' s(\lambda - \lambda') \\ \times \ln \left\{ [1 + \eta_{n-1}(\lambda')] [1 + \eta_{n+1}(\lambda')] \right\}, \qquad n = 1, 2, \dots,$$
(19.84)

where $\eta_0(\lambda) \equiv 0$. These equations are complemented by the leading asymptotic

$$\lim_{n \to \infty} \frac{\ln \eta_n(\lambda)}{n} = \frac{2h}{T}.$$
(19.85)

The free energy per site is expressible in two equivalent forms

$$f = -2sh - T\sum_{n=1}^{\infty} \int_{-\infty}^{\infty} d\lambda \, a_n(\lambda) \ln\left[1 + \eta_n^{-1}(\lambda)\right], \qquad (19.86)$$

$$f = e_0 - T \int_{-\infty}^{\infty} \mathrm{d}\lambda \, s(\lambda) \ln[1 + \eta_1(\lambda)], \qquad (19.87)$$

where

$$e_0 = -2\pi \int_{-\infty}^{\infty} \mathrm{d}\lambda \, s(\lambda) a_{2s}(\lambda) \tag{19.88}$$

is the specific free energy at T = 0, i.e. the ground-state energy per site.

19.4 Ground state, low-lying excitations and low-temperature properties

In the limit $T \to 0$, the TBA equations (19.84) for the energy functions $\epsilon_n(\lambda) = T \ln \eta_n(\lambda)$ take the form

$$\epsilon_{n}(\lambda) = -2\pi s(\lambda)\delta_{n,2s} + T \int_{-\infty}^{\infty} d\lambda' \, s(\lambda - \lambda') \\ \times \ln\left[\left(1 + e^{\epsilon_{n-1}(\lambda')/T} \right) \left(1 + e^{\epsilon_{n+1}(\lambda')/T} \right) \right]$$
(19.89)

with $\epsilon_0(\lambda) \to -\infty$. The asymptotic condition (19.85) is equivalent to $\lim_{n\to\infty} \epsilon(\lambda)/n = 2h$. It follows from the form of the TBA equations that $\epsilon_n(\lambda) \ge 0$ for $n \ne 2s$ while the function $\epsilon_{2s}(\lambda)$ can have either sign.

At T = 0 and for h = 0, we have the solution

$$\epsilon_n^{(0)}(\lambda) = -2\pi s(\lambda)\delta_{n,2s} = -\frac{\pi}{\cosh(\pi\lambda)}\delta_{n,2s}.$$
(19.90)

Forming the convolution of Eq. (19.80) with the inverse function A^{-1} and using the TBA equations (19.89), we obtain

$$\rho_n^{(0)}(\lambda) = s(\lambda)\delta_{n,2s}, \qquad \tilde{\rho}_n^{(0)}(\lambda) = 0.$$
 (19.91)

The ground state of the Hamiltonian H^s is thus described as the unperturbed Dirac sea of 2sstrings. The total z-component of the spin in this state is given by

$$\frac{\langle S^z \rangle}{N} = s - \sum_{n=1}^{\infty} n \int_{-\infty}^{\infty} \mathrm{d}\lambda \,\rho_n^{(0)}(\lambda) = 0, \tag{19.92}$$

i.e. for the chain of N sites there is just $M_{2s} = N/2$ strings of length 2s and $M_n = 0$ for $n \neq 2s$, so that M = sN. Using the relations (19.77) and (19.81), the ground-state energy per site (19.88) is expressible as follows

$$e_0 = -\int_{-\infty}^{\infty} \mathrm{d}\lambda \, s(\lambda) \sum_{l=1}^{2s} \frac{\mathrm{d}}{\mathrm{d}\lambda} \theta_{2l-1}(\lambda), \qquad \frac{\mathrm{d}\theta_n(\lambda)}{\mathrm{d}\lambda} = \frac{n}{\lambda^2 + \frac{n^2}{4}}.$$
(19.93)

The integral can be evaluated by using the formula [5]

$$\int_{-\infty}^{\infty} \mathrm{d}\lambda \, \frac{1}{2\cosh(\pi\lambda)} \frac{1}{\lambda^2 + b^2} = \frac{1}{b}\beta\left(b + \frac{1}{2}\right) \qquad (b > 0),\tag{19.94}$$

where $\beta(n) = \int_0^1 \mathrm{d}t \, t^{n-1}/(1+t)$ is the beta function. For integer n, it is given by

$$\beta(n) = (-1)^{n+1} \ln 2 + \sum_{l=1}^{n-1} \frac{(-1)^{n+l+1}}{l}.$$
(19.95)

Thus,

$$e_0 = -2\sum_{n=1}^{2s} \beta(n) = \begin{cases} -\sum_{n=1}^{s} \frac{2}{2n-1} & \text{integer } s, \\ -2\ln 2 + \sum_{n=1}^{s-\frac{1}{2}} \frac{1}{n} & \text{half-integer } s. \end{cases}$$
(19.96)

The structure of low-lying excitations is the following. The simplest are the hole excitations in the Dirac sea of 2s strings which are created by taking a string with center λ to $\lambda \to \infty$. The relative energy and momentum with respect to the ground state are

$$\Delta E(\lambda) = \frac{\pi}{\cosh(\pi\lambda)}, \qquad K(\lambda) = \frac{\pi}{2} - \arctan[\sinh(\pi\lambda)], \qquad (19.97)$$

so the dispersion relation reads

$$\Delta E(K) = \pi |\sin K|. \tag{19.98}$$

This relation does not depend on s and coincides with the spin-1/2 dispersion result (15.84). The energy spectrum is gapless. There are other low-lying excitations which have no counterparts in the spin-1/2 case [50]:

- M = sN 1, $M_{2s} = \frac{1}{2}N 1$, $M_{2s-1} = 1$, all other $M_n = 0$; the spin of this state is 1.
- $M = sN, M_{2s} = \frac{1}{2}N 2, M_{2s-1} = M_{2s+1} = 1$, all other $M_n = 0$; this state has spin 0.

In both cases, the excitation energy and momentum are given additively by the energies and momenta (19.97) of individual holes. The contribution of *n*-strings with $n \neq 2s$ to dynamical quantities vanishes, their role reduces itself to distinguishing the states of different spins.

It is instructive to comment the nature of low-lying excitation spectrum for the general isotropic spin-1 chain with the Hamiltonian

$$H^{1} = \frac{1}{2} \sum_{n=1}^{N} \left[\mathbf{S}_{n} \cdot \mathbf{S}_{n+1} - \delta \left(\mathbf{S}_{n} \cdot \mathbf{S}_{n+1} \right)^{2} \right], \qquad \mathbf{S}_{N+1} \equiv \mathbf{S}_{1}.$$
(19.99)

The present case (19.72) corresponds to $\delta = 1$ and its energy spectrum is gapless. The case $\delta = -1$ is also solvable by using the Bethe-ansatz method [57] and it exhibits the gapless spectrum as well. The ground state is known at the point $\delta = -1/3$ [58, 59] and the spectrum has a gap. Numerical methods [60] indicate that the spectrum has a gap in the whole region $-1 < \delta < 1$. The point $\delta = 0$ is of special interest as a test for the Haldane prediction [61, 62]: the antiferromagnetic chain Hamiltonian $\sum_{n=1}^{N} \mathbf{S}_n \cdot \mathbf{S}_{n+1}$ has an energy gap for integer s and is gapless for half-integer s (like in the s = 1/2 case).

At T = 0 and for h > 0, the rapidities are constrained to the interval $\langle -b, b \rangle$ where $b \to \infty$ as $h \to 0$. We can perform the Wiener-Hopf analysis of the corresponding integral equations for the density $\rho(\lambda)$, in close analogy with Sect. 14. To leading order in h, the final result for the ground-state energy per site $e_0(h)$ and the magnetic susceptibility χ is [52]

$$e_0(h) = e_0 - \frac{2s}{\pi^2}h^2, \qquad \chi = \frac{4s}{\pi^2}.$$
 (19.100)

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Based on the formalism similar to that developed in Sect. 16, the low-temperature behavior of the specific heat at h = 0 was obtained in the form

$$\frac{C^s}{T} = \frac{1}{3} - \frac{1}{\pi^2} \sum_{n=1}^{2s-1} \int_0^{1/x_n^2} \mathrm{d}x \, \left[\frac{1}{x} \ln(1-x) + \frac{1}{1-x} \ln x \right], \tag{19.101}$$

where

$$x_n = \sin \frac{\pi(n+1)}{2(s+1)} \left[\sin \frac{\pi}{2(s+1)} \right]^{-1}.$$
(19.102)

For s = 1/2 we obtain $C^{\frac{1}{2}} = T/3$ as in (16.116), for s = 1 we have $C^{1} = T/2$, etc.

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