

# The Spin-1/2 XXZ Chain at Finite Magnetic Field: Crossover Phenomena Driven by Temperature<sup>1</sup>

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We investigate the asymptotic behaviour of spin-spin correlation functions for the integrable Heisenberg chain. To this end we use the Quantum Transfer Matrix (QTM) technique developed in ref. 1) which results in a set of non-linear integral equations (NLIE). In the case of the largest eigenvalue the solution to these equations yields the free energy and by modifications of the paths of integration the next-leading eigenvalues and hence the correlation lengths are obtained. At finite field  $h > 0$  and sufficiently high temperature  $T$  the next-leading eigenvalue is unique and given by a 1-string solution to the QTM taking real and negative values thus resulting into exponentially decaying correlations with antiferromagnetic oscillations. At sufficiently low temperatures a different behaviour sets in where the next-leading eigenvalues of the QTM are given by a complex conjugate pair of eigenvalues resulting into incommensurate oscillations. The above scenario is the result of analytical and numerical investigations of the QTM establishing a well defined crossover temperature  $T_c(h)$  at which the 1-string eigenvalue to the QTM gets degenerate with the 2-string solution. Among other things we find a simple particle-hole picture for the excitations of the QTM allowing for a description by the dressed charge formulation of CFT.

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**KEY WORDS:** Exact solution; quantum transfer matrix; strongly correlated systems; crossover phenomena; level crossing; conformal field theory.

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<sup>1</sup> Dedicated to Professor Rodney Baxter on the occasion of his 60th birthday.

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## 1. INTRODUCTION

In this contribution we report on a new crossover phenomenon observed in the longitudinal correlation function at finite magnetic field  $h$  and finite temperature  $T$  of the  $XXZ$  spin-chain with anisotropy parameter  $0 < \Delta < 1$ .

As is well known any thermodynamic quantity derived from the free energy of the one-dimensional  $XXZ$  model is an analytic function of finite  $h$  and  $T$ . Phase transitions and associated mathematical singularities may and do occur in the ground state, i.e., at  $T=0$ . However, quantities not obtained from the free energy, but characterising the asymptotics of correlation functions may show “their own” non-analyticities at finite temperatures. Indeed the  $XXZ$  chain in an external magnetic field does show well defined non-analyticities in the *correlation lengths* of the longitudinal spin-spin correlation functions. We want to point out that these crossover phenomena are a result of strong correlations and finite temperature. The crossover does not take place for the case  $\Delta=0$  corresponding to free fermions.

For the attractive regime  $-1 < \Delta \leq 0$  of the  $XXZ$  chain the investigations are not yet carried out for finite field  $h$  and finite  $T$ . Here the physical phenomena are expected to be much richer. Even for the case of vanishing magnetic field  $h=0$  a sequence of crossovers (commensurate-incommensurate-commensurate) for an increase of  $T$  from 0 to  $\infty$  was found.<sup>(2)</sup>

The method we apply (as that used in ref. 2) is based on a mapping of the  $XXZ$  chain at finite temperatures onto a classical model in two dimensions and the formulation of a suitable quantum transfer matrix (QTM) describing the transfer along the chain. The spectrum of the QTM succumbs to a Bethe ansatz (BA) treatment and the corresponding BA equations can be cast into the form of non-linear integral equations. Crossover phenomena of correlation lengths manifest themselves as level crossings of next-leading eigenvalues of the QTM. At finite field  $h > 0$  and sufficiently high temperature the relevant eigenvalues for the longitudinal correlation functions are 1-string and 2-string solutions (both solutions belong to the  $S=0$  sector of the model). The truly next-leading eigenvalue is unique and given by the 1-string solution to the QTM taking real and negative values thus resulting into exponentially decaying correlations with antiferromagnetic oscillations. In some sense at sufficiently high temperature the properties of the system are determined by the longitudinal (“classical”) terms of the Hamiltonian, i.e., the  $S^z S^z$  coupling and the field in  $z$  direction, which dominate over the transversal exchange (“quantum mechanical”) terms. At sufficiently low temperature a different behavior is expected on grounds of predictions by conformal field theory (CFT).<sup>(3,4)</sup> In particular, correlations with incommensurate  $2k_F$  oscillations are expected.<sup>(5,6)</sup>

As a consequence of this, the QTM has to develop complex conjugate pairs of eigenvalues at sufficiently low temperatures. This scenario has not been investigated before. The purpose of this contribution is to present the first “Bethe ansatz” study of this crossover phenomenon and to provide reasonably accurate values for the crossover temperature  $T_c$ . As pointed out already, for the free fermion case  $T_c = \infty$ , i.e., the crossover does not take place. In physical terms this may be understood in the way that due to the absence of longitudinal couplings the longitudinal terms never dominate over the transversal terms.

This report is organized as follows. In Section 2 we introduce some basic definitions of the XXZ chain and present its properties at low temperature as obtained within conformal field theory (CFT). In Section 3 the approach to thermodynamic properties by use of a lattice path integral formulation and the quantum transfer matrix (QTM) is reviewed. In particular the set of non-linear integral equations for the two auxiliary functions  $a(x)$  and  $\bar{a}(x)$  corresponding to the energy density functions of spinons with spin  $\pm 1/2$  are given. In Section 4 numerical results are given for the correlation length and Fermi momentum of the longitudinal spin-spin correlation function. Finally, the particle-hole picture resulting at low temperatures is discussed. A complete exposition of how this is related to the dressed charge formulation of CFT will appear in ref. 7.

## 2. ANISOTROPIC HEISENBERG MODEL

The XXZ model is defined by the Hamiltonian

$$H = J \sum_{\langle i, j \rangle} [S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z] - h \sum_j S_j^z \quad (1)$$

where  $J > 0$ ,  $h > 0$  and  $S^{x, y, z}$  are spin-1/2 operators. For  $T = 0$  the system is in one of three phases. For anisotropy parameter  $|\Delta| > 1$  we have two ordered phases and for  $|\Delta| \leq 1$  a critical phase. In the latter case the anisotropy parameter is conveniently parameterized by  $\Delta = \cos \gamma$ . In the following we take  $0 < \gamma < \pi/2$  (repulsive regime) for simplicity. The excitations are gapless spinons with spin 1/2

$$\varepsilon_F(k) = v \sin k, \quad 0 \leq k \leq \pi \quad (2)$$

$$v = \frac{\sin \gamma}{\gamma} \pi J \quad (3)$$

At zero temperature the spin correlations decay algebraically,<sup>(8-12)</sup> with exponents depending on the magnetic field in a nontrivial way.<sup>(6)</sup> At finite temperature the correlations decay exponentially  $e^{-r/\xi}$  with in general different correlation lengths  $\xi$  for different correlation functions. At low temperatures the correlation lengths can be related by conformal mappings to the scaling dimensions  $x$  of the fields at  $T=0$

$$\xi = \frac{v}{2\pi x T} \quad \text{for } T \ll 1$$

The scaling dimensions  $x$  are calculated from finite size corrections to the energy levels of the Hamiltonian and scaling predictions by CFT

$$E_x - E_0 = \frac{2\pi}{L} v(x + N^+ + N^-) + o\left(\frac{1}{L}\right) \quad (4)$$

where  $N^+$  and  $N^-$  are integers labelling the conformal tower. The critical exponents of the spin-1/2  $XXZ$  model are those of a  $c=1$  Gaussian theory. At zero magnetic field the exponents are given in terms of the anisotropy parameter  $\gamma$

$$x = \frac{1 - \gamma/\pi}{2} S^2 + \frac{1}{2(1 - \gamma/\pi)} m^2 \quad (5)$$

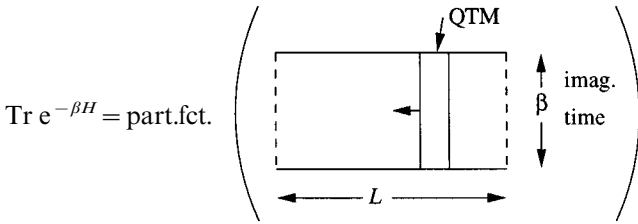
where  $S$  and  $m$  are integers corresponding to the  $S^x$  component of the state and the number of excitations from the left to the right Fermi point, respectively. The longitudinal correlation is

$$\langle S_0^z S_r^z \rangle \simeq C_1 \frac{\cos(2k_F r)}{r^{1/(1 - \gamma/\pi)}} - \frac{C_2}{r^2} \quad (6)$$

where  $C_1$  and  $C_2$  do not depend on the distance  $r$ . For zero magnetic field the Fermi momentum  $k_F$  is equal to  $\pi/2$ . For finite magnetic field and temperature we expect a deviation of  $x$  and  $k_F$  from the above quoted values.

### 3. FINITE TEMPERATURES

The properties of the quantum system at finite temperature are determined within a path integral formulation. The partition function of the 1d quantum system at finite temperature is mapped to that of a 2d classical system pictorially represented by



For the classical system we can choose a suitable transfer approach. The quantum transfer matrix (QTM), i.e., the column-to-column transfer matrix, possesses a unique largest eigenvalue and a spectral gap to the next-leading eigenvalues which persists even in the limit of infinite Trotter number as long as the temperature is finite.<sup>(13-18)</sup> Hence the free-energy and correlation lengths are simply determined from the largest  $A_0$  and next largest eigenvalues  $A_j$  of the QTM

$$f = -\frac{1}{\beta} \lim \ln A_0 \tag{7}$$

$$C(r) = A_1 \left(\frac{A_1}{A_0}\right)^r + A_2 \left(\frac{A_2}{A_0}\right)^r + \dots$$

with coefficients  $A_1, A_2$  given by matrix elements. The diagonalization of the QTM can be performed by means of a Bethe ansatz resulting into eigenvalue equations of the form of Baxter's  $A - q$  equation. For finite Trotter number  $N$  we find

$$A(x) q(x) = e^{-\beta h/2} \Phi(x - i\gamma/2) q(x + i\gamma) + e^{+\beta h/2} \Phi(x + i\gamma/2) q(x - i\gamma) \tag{8}$$

where

$$\Phi(x) = [\sinh(x - ix_0) \sinh(x + ix_0)]^{N/2}, \quad x_0 := \frac{\gamma}{2} - \frac{\beta}{N} \tag{9}$$

$$q(x) = \prod_j \sinh(x - x_j)$$

The roots  $x_j$  are determined from the Bethe ansatz equation

$$p(x_j) = -1, \quad \text{where } p(x) := e^{-\beta h} \frac{\Phi(x - i\gamma/2) q(x + i\gamma)}{\Phi(x + i\gamma/2) q(x - i\gamma)} \tag{10}$$

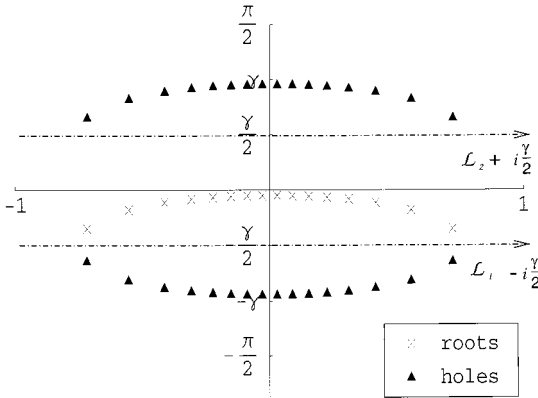


Fig. 1. Distribution of roots and holes for the largest eigenvalue for anisotropy parameter  $\gamma = \pi/3$ , reciprocal temperature  $\beta = 12$  and  $h = 0.6$ . Note that straight contours with imaginary parts  $\pm\gamma/2$  separate the roots from the holes. The contours  $\mathcal{L}_1 - i\gamma/2$  and  $\mathcal{L}_2 + i\gamma/2$  are depicted by dashed-dotted lines. Note that roots and holes get arbitrarily close to  $\mathcal{L}_1 - i\gamma/2$  for low temperatures  $T$  and positive  $h$ .

thus rendering  $A(x)$  analytic. We like to note that in general there are more solutions to the Bethe ansatz equation  $p(x) = -1$  than roots  $x_j$ . The additional solutions are called *holes*. For an illustration of a typical case see Fig. 1.

The corresponding distributions of roots and holes remain discrete even in the limit of infinite Trotter number  $N \rightarrow \infty$ . The method of studying these equations was developed in ref. 1 and results into two equations for two auxiliary functions  $\alpha(x) := 1/p(x - i\gamma/2)$  and  $\bar{\alpha}(x) := p(x + i\gamma/2)$  (corresponding to  $S = 1/2$  spinon and antispinon dressed energy functions)

$$\ln \alpha(x) = -\frac{v\beta}{\cosh \frac{\pi}{\gamma} x} + \frac{\pi\beta h}{2(\pi - \gamma)} + [\kappa *_{1} \ln(1 + \alpha)](x) - [\kappa *_{2} \ln(1 + \bar{\alpha})](x - i\gamma + i\epsilon) \quad (11)$$

An analogous integral equation for  $\bar{\alpha}$  can be obtained from the above one by use of the obvious identity  $\ln \bar{\alpha}(x) = -\ln \alpha(x + i\gamma)$  thus completing the non-linear integral equations. The integral kernel  $\kappa(x)$  is defined by a Fourier integral

$$\kappa(x) := \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\sinh\left(\frac{\pi}{2} - \gamma\right) k \cos(kx)}{2 \cosh \frac{\gamma}{2} k \sinh \frac{\pi - \gamma}{2} k} dk \quad (12)$$

The symbol  $*_{\mathcal{L}}$  denotes convolution

$$f * g(x) = \int_{\mathcal{L}} f(x-y) g(y) dy \tag{13}$$

with a suitably defined integration contour  $\mathcal{L}$ . In (11) the subscripts  $*_1$  ( $*_2$ ) refer to integration paths  $\mathcal{L}_1$  and  $\mathcal{L}_2$  that extend from  $-\infty$  to  $+\infty$  and lie below the distribution of numbers  $x_j + i\gamma/2$  and above  $x_j - i\gamma/2$ . An additional and last requirement for these paths is that all roots  $x_j$  be

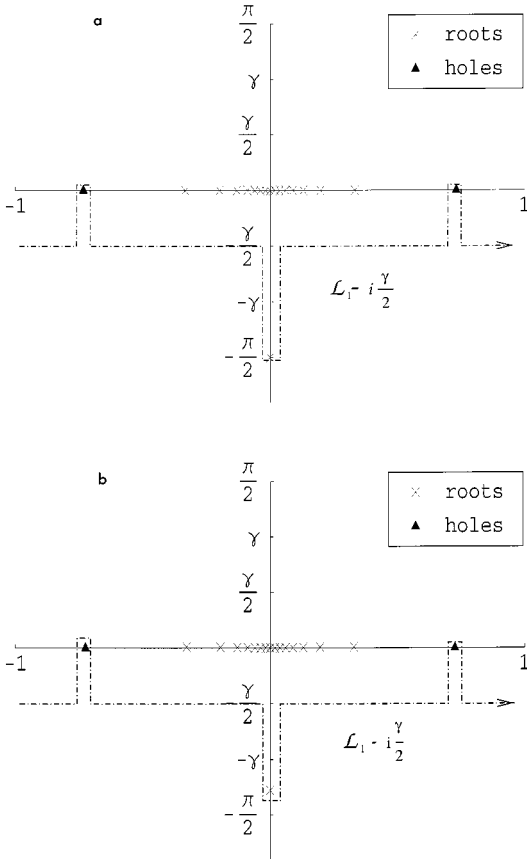


Fig. 2. Distribution of roots and holes for a 1-string solution for anisotropy parameter  $\gamma = \pi/3$ , reciprocal temperature  $\beta = 3.0$ , and (a)  $h = 0$  and (b)  $h = 0.6$ . Of all hole solutions only the two new holes close to the real axis are shown. Note that for (a) the 1-string is situated exactly at  $-i\pi/2$  and the holes lie on the real axis. For positive magnetic field (b) the 1-string is shifted upwards (see also Fig. 4). The contour  $\mathcal{L}_1 - i\gamma/2$  is depicted by a dashed-dotted line.

situated between  $\mathcal{L}_1 - i\gamma/2$  and  $\mathcal{L}_2 + i\gamma/2$ , but no hole solution to the Bethe ansatz equation.

For the largest eigenvalue the distribution of roots and holes is depicted in Fig. 1. Here the paths  $\mathcal{L}_1 - i\gamma/2$  and  $\mathcal{L}_2 + i\gamma/2$  are just straight lines with imaginary parts  $\mp \gamma/2$ . Hence,  $\mathcal{L}_{1,2}$  coincide with the real axis.

The cases of next-leading excitations which are of 1-string type (root  $y_0$  in the lower half plane) and 2-string type (upper and lower roots  $y_+$  and  $y_-$  separated by approximately  $i\gamma$ ) are shown in Figs. 2 and 3. For the excited states the contours of integration are deformed. Only the path

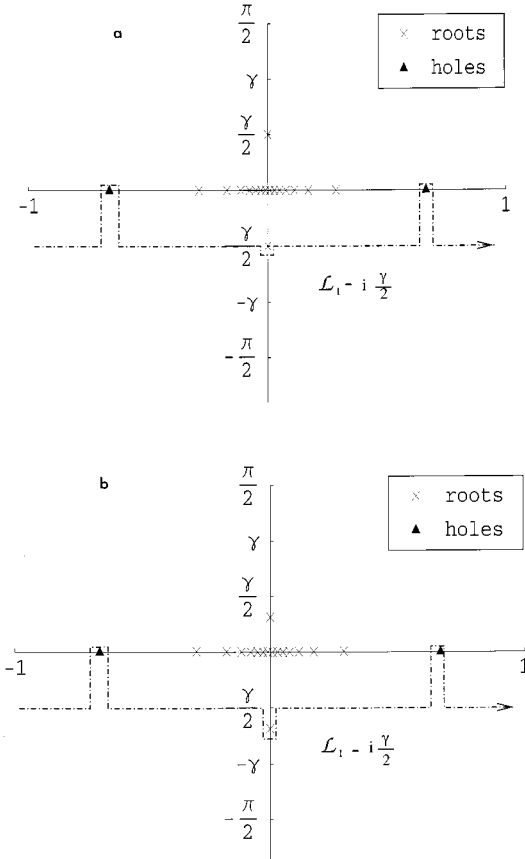


Fig. 3. Distribution of roots and holes for a 2-string solution for anisotropy parameter  $\gamma = \pi/3$ , reciprocal temperature  $\beta = 3.0$ , and (a)  $h = 0$  and (b)  $h = 0.6$ . Only the two new holes close to the real axis are shown. Note that for (a) the 2-string is symmetric with respect to the real axis and situated approximately at  $\pm i\gamma/2$ ; the holes lie on the real axis. For positive magnetic field (b) the 2-string is shifted downwards (see also Fig. 4). The contour  $\mathcal{L}_1 - i\gamma/2$  is depicted by a dashed-dotted line.



$\mathcal{L}_1 - i\gamma/2$  is shown explicitly,  $\mathcal{L}_2 + i\gamma/2$  is simpler as it is mostly following a straight line with imaginary part  $+\gamma/2$  with loop in counter clockwise manner around  $y_0 + i\gamma$  and  $y_- + i\gamma$ , respectively.

The contours may be straightened and by use of Cauchy's theorem we pick up residues that lead to additive contributions to the driving terms in the non-linear integral equations.<sup>(1)</sup> This form of the NLIE is particularly useful for numerical treatments.<sup>(7)</sup>

Finally, the subsidiary conditions  $\alpha(y_0 + i\gamma/2) = -1$  and  $\alpha(y_{\pm} + i\gamma/2) = -1$  with  $y_0, y_+$  and  $y_-$  denoting the root of the 1-string and the upper and lower constituents of the 2-string, respectively, yield the information on the positions of the string parameters.

The eigenvalues of the QTM are expressed in terms of  $\alpha(x), \bar{\alpha}(x)$

$$\ln A = -\beta e_0 + \frac{1}{2\gamma} \int \frac{\ln[(1 + \alpha(x))(1 + \bar{\alpha}(x))]}{\cosh \frac{\pi}{\gamma} x} dx \quad (14)$$

where  $e_0$  is the groundstate energy for zero magnetic field and the integration contours are  $\mathcal{L}_{1,2}$ . However, due to certain analyticity properties of the integrand these contours can be simplified to just one contour along the real axis, surrounding the numbers  $\theta + i\gamma/2$  in clockwise manner where  $\theta$  is any of the hole solutions to the Bethe ansatz equation close to the real axis.

The range of validity (convergence) of the integral equation (11) for  $\alpha(x)$  is the strip  $\text{Im}(x) \in [0, \gamma]$ . Sometimes it is necessary to extend the above equation to the strip  $\text{Im}(x) \in [-(\pi - \gamma), 0]$ , e.g., for calculating  $\alpha(y_0 + i\gamma/2) = -1$  with  $y_0$  in the lower half plane, see Fig. 2. One version of such an expression for the 1-string pattern is

$$\begin{aligned} \ln \alpha(x) = & \frac{\pi\beta h}{\pi - \gamma} - [r * \ln(1 + \alpha)](x) + [r * \ln(1 + \bar{\alpha})](x - i\gamma) \\ & + \log \left[ \frac{\sinh \frac{\pi}{\pi - \gamma} (x - y_0 - i3\gamma/2)}{\sinh \frac{\pi}{\pi - \gamma} (x - y_0 + i\gamma/2)} \prod_{j=1,2} \frac{\sinh \frac{\pi}{\pi - \gamma} (x - \theta_j + i\gamma/2)}{\sinh \frac{\pi}{\pi - \gamma} (x - \theta_j - i\gamma/2)} \right] \end{aligned} \quad (15)$$

where

$$r(x) = \frac{i}{2(\pi - \gamma)} \left( \coth \frac{\pi}{\pi - \gamma} x - \coth \frac{\pi}{\pi - \gamma} (x + i\gamma) \right) \quad (16)$$

Note that the above expression for  $\alpha(x)$  is valid for  $x$  below the real axis, however  $\alpha, \bar{\alpha}$  on the right hand side are evaluated for strictly real arguments, i.e.,  $*$  denotes standard convolution with the integration contour along the real axis. In particular, there are no deformations of the contour as discussed above. They have been removed by use of Cauchy's theorem. In turn, the rapidities  $\theta_1, \theta_2$  and the 1-string parameter  $y_0$  show up explicitly. Note that the corresponding expression for the 2-string pattern is obtained by simply exchanging  $y_0$  with  $y_-$  (the lower part of the 2-string). In this case, the upper part  $y_+$  does not appear explicitly. The details will be presented in ref. 7.

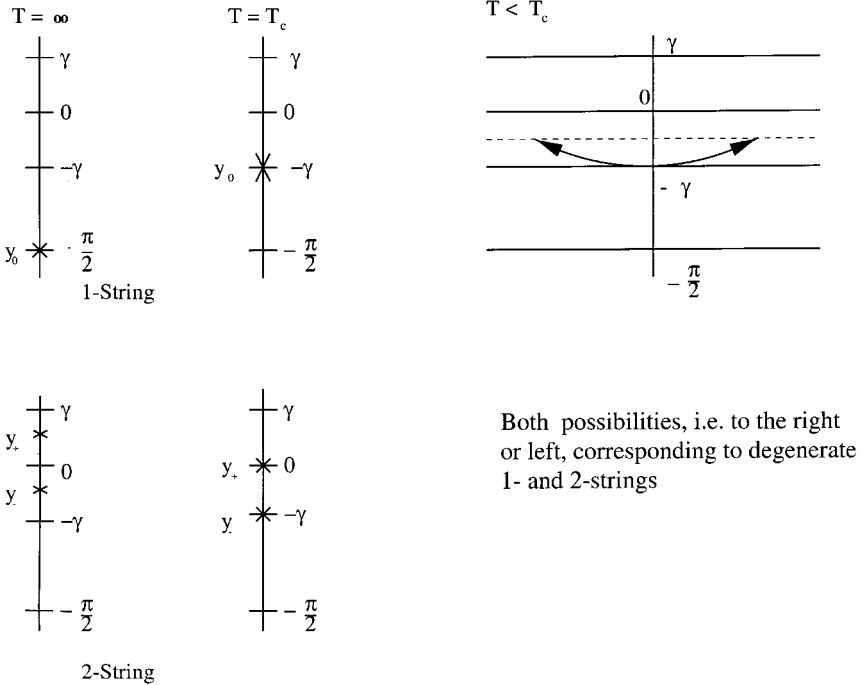
#### 4. CROSSOVER SCENARIO AND THE PARTICLE-HOLE PICTURE

From the next-largest eigenvalue(s)  $A_1$  of the QTM the asymptotic behavior of the correlation functions is determined. If  $A_1$  is real and positive (negative), the decay is purely exponential without (with) sublattice oscillations. In general  $A_1$  may be complex and the asymptotics are characterized by a finite correlation length  $\xi$  and Fermi-momentum  $k_F$  defined by

$$\frac{A_1}{A_0} = e^{-1/\xi \pm i2k_F}$$

We have numerically solved the nonlinear integral equations for the next-leading eigenvalue(s) and plot the results in Figs. 4 and 5.

Summarizing our results we see that the previously drawn picture of excitations of distinctly 1-string and 2-string type is valid only for  $h=0$  or, if  $h>0$  for sufficiently high  $T$ . For this case the 1-string solution dominates and the eigenvalue is real because of the left-right symmetry of the Bethe ansatz pattern. The 2-string solution is subdominant. Both strings lie on the imaginary axis where for  $T=\infty$  the 1-string is located at  $-i\pi/2$  and the 2-string is symmetric with respect to the real axis. For decreasing temperature we observe a characteristic motion of the 1-string upwards and the 2-string downwards along the imaginary axis, cf. Fig. 4. This motion continues until the root of the 1-string ( $y_0$ ) and the lower root of the 2-string ( $y_-$ ) take identical values. The corresponding temperature defines  $T_c$ . For lower temperatures a horizontal motion sets in. The considered root previously on the imaginary axis develops a non-vanishing real part which may be positive or negative, see Fig. 4. The corresponding Bethe ansatz patterns are related by reflection at the imaginary axis, the corresponding



Both possibilities, i.e. to the right or left, corresponding to degenerate 1- and 2-strings

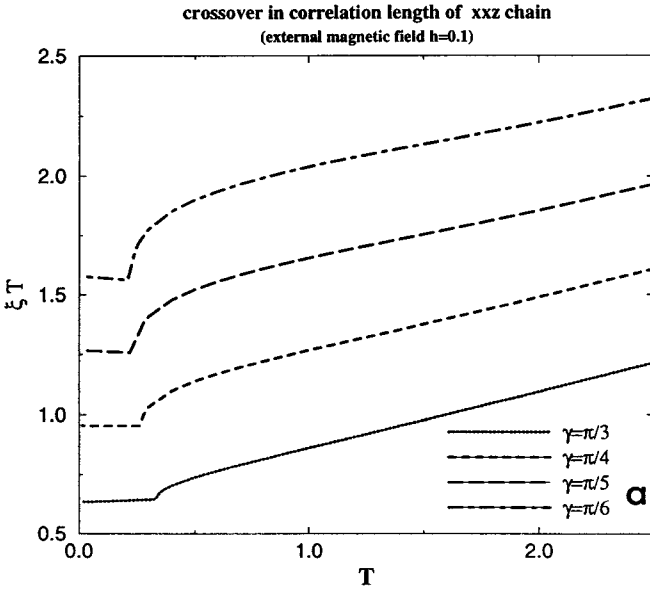
Fig. 4. Schematic depiction of the crossover scenario. At the left we show for the 1-string and 2-string solutions how the strings move away from their high temperature positions upon a decrease of  $T$ . At some well-defined temperature  $T_c$  both solutions become degenerate. A further decrease of temperature forces the 1-string and the lower part of the 2-string to move away from the imaginary axis. As a result we have two complex conjugate solutions with complex eigenvalues.

eigenvalues are complex conjugate. There is no longer any qualitative distinction like for temperatures higher than  $T_c$ .

The reason for this crossover may be understood qualitatively in the following way. The subsidiary condition for the 1-string  $y_0$  (or for the 2-string with  $y_0$  replaced by  $y_-$ ) is  $\alpha(y_0 + i\gamma/2) = -1$  which yields due to (15)

$$\frac{\pi\beta h}{\pi - \gamma} + \log \left[ \frac{\sinh \frac{\pi}{\pi - \gamma} (y_0 - \theta_1 + i\gamma) \sinh \frac{\pi}{\pi - \gamma} (y_0 - \theta_2 + i\gamma)}{\sinh \frac{\pi}{\pi - \gamma} (y_0 - \theta_1) \sinh \frac{\pi}{\pi - \gamma} (y_0 - \theta_2)} \right]$$

= "integral expressions" (17)



**deviation from  $2k_F = \pi$  oscillations**

(external magnetic field  $h=0.1$ )

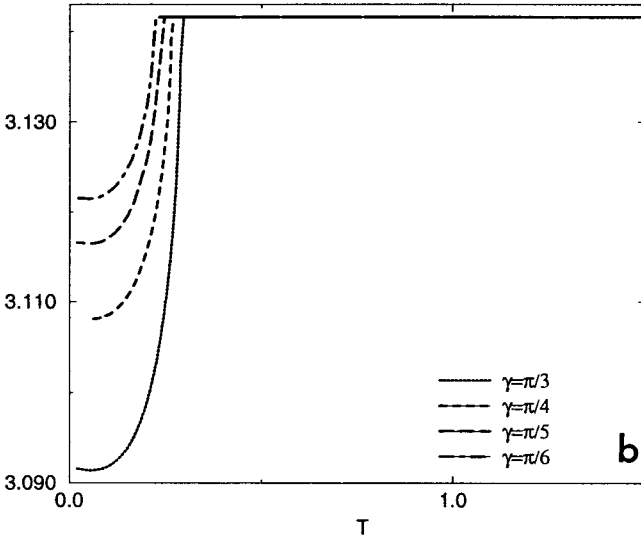


Fig. 5. The  $XXZ$  chain for finite field  $h = 0.1$  and several values of the anisotropy parameter  $\gamma$ . Temperature dependence of: (a) longitudinal correlation length  $\xi$  times  $T$ , (b) Fermi-momentum. The crossover temperature is monotonously decreasing for decreasing  $\gamma$  with a seemingly finite limiting value for  $\gamma \rightarrow 0$ .

Unfortunately, the right hand side has to be evaluated numerically. It turns out to be of order  $O(\beta h)$ , but smaller than the first term on the left hand side. In any case, the equation (17) for  $y_0$  has two inequivalent solutions. These solutions are purely imaginary and different for small  $\beta h$  ( $\leftrightarrow$  distinct 1- and 2-strings); they have same imaginary part but non-vanishing real parts with opposite signs for large  $\beta h$  ( $\leftrightarrow$  degenerate 1- and 2-strings). The crossover is typically associated with square root singularities. The precise value of  $T_c$  can only be calculated numerically.

The results for the correlation length and Fermi momentum are shown in Fig. 5. Most strikingly we see a non-analytic temperature dependence for non-vanishing external magnetic fields at the well-defined crossover temperature  $T_c$ ! The singularity at  $T_c$  is of square root type. Most significant is the non-analytic behaviour of the Fermi momentum. At low temperature the oscillations are incommensurate and at zero temperature the Fermi momentum  $k_F$  and magnetization  $m$  are strictly related by  $k_F = (1/2 - m)\pi$ , a relation which ceases to hold at elevated temperatures. At sufficiently high temperatures the oscillations are commensurate with  $k_F = \pi/2$ . The loss of the left-right symmetry in the Bethe ansatz patterns at low temperatures is the reason for the incommensurability of  $k_F$  and the non-analytic behavior of the correlation length.

We note that temperature and magnetic field act in roughly opposite ways which can be inferred in part from their appearance in the combination  $h/T$  in the NLIE. At sufficiently low temperatures the distinguishing characters of the 1-string and 2-string disappear completely and a root-hole picture emerges as shown in Fig. 6. Here the relevant modifications of the excited state of the QTM in comparison to the ground state (see Fig. 1)

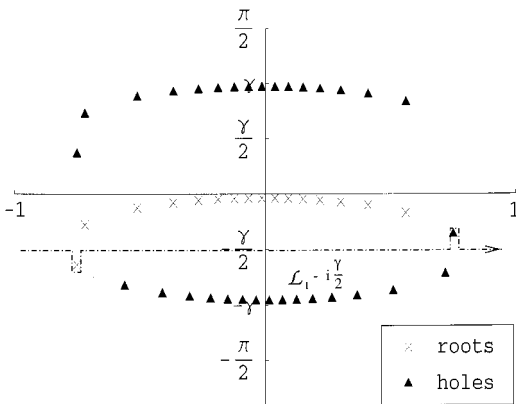


Fig. 6. Bethe ansatz pattern at low temperature ( $h=0.6$  and  $\beta=12.0$ ) corresponding to a 1-string (or 2-string) solution at sufficiently high temperature.

can be characterized as a rearrangement of the roots and holes on an ellipsoidal curve. Clearly, the same constructions and terminology as used for the excitations of Fermi systems applies. In this finite field case ( $h > 0$ ), the analytic treatment of the low-temperature asymptotics not only confirms the predictions of CFT, but also recovers completely the dressed charge formalism as will be shown in ref. 7.

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