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The free energy singularity of the asymmetric six-vertex model and the excitations of the asymmetric XXZ chain

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Abstract

We consider the asymmetric six-vertex model, widely used to describe the equilibrium shape of crystals, and the relevant asymmetric XXZ chain. By means of the Bethe-ansatz solution we determine the free energy singularity, as function of the external field, at two special points on the phase boundary. We confirm the exponent $\frac{3}{2}$ (checked experimentally), as the antiferroelectric ordered phase is reached from the incommensurate phase normally to this boundary, and we determine a new singularity along the tangential direction. Both singularities describe the rounding off of the crystal near a facet. At this point the hole excitations of the spin chain show dispersion relations $\Delta E \sim (\Delta P)^{1/2}$ at small momenta, leading to a finite-size scaling $\Delta E \sim N^{-1/2}$ for the low-lying excited states, N being the chain size. We discuss the nature of the phase transition and the behavior of arrow-arrow correlation lengths in the ordered phase. © 1997 Published by Elsevier Science B.V.

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1. Introduction

After the pioneering paper of Yang, Yang and Sutherland [1] the asymmetric six-vertex model, i.e. the symmetric six-vertex model in a field, was recently rediscovered because of its connection to a number of physically interesting problems, first among

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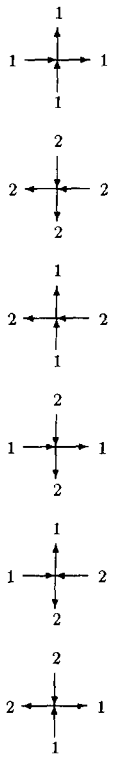

$$= e^{h+v}\,\frac{\sinh(\gamma-u)}{\sinh\gamma} = e^{\beta(\delta/2-\epsilon)+h+v} = R^{11}_{11}(u)$$

$$= e^{-h-v}\,\frac{\sinh(\gamma-u)}{\sinh\gamma} = e^{\beta(\delta/2-\epsilon)-h-v} = R^{22}_{22}(u)$$

$$= e^{-h+v}\,\frac{\sinh u}{\sinh\gamma} = e^{\beta(-\delta/2-\epsilon)-h+v} = R^{22}_{11}(u)$$

$$= e^{h-v}\,\frac{\sinh u}{\sinh\gamma} = e^{\beta(-\delta/2-\epsilon)+h-v} = R^{11}_{22}(u)$$

$$= 1 = 1 = R^{12}_{21}(u)$$

$$= 1 = 1 = R^{21}_{12}(u)$$

Fig. 1. Boltzmann weights in the notation with spectral parameter u compared to that of Ref. [9]. The physical region is $0 < u < \gamma$.

them the determination of the shape of a crystal at equilibrium with its vapor phase [2–4]. This can be achieved by mapping the asymmetric six-vertex onto, say, the (001) facet of a bcc crystal under the condition that no overhangs or voids are allowed (see e.g. Refs. [2,3,5] for details on the mapping). Excitations in the vertex model correspond to small tilts away from the (001) facet [5] and it can be shown [6] that the free energy as function of the two components of the field gives exactly the equilibrium shape of the crystal.

In its own right, the asymmetric six-vertex model provides an interesting two-dimensional system of interacting dipoles in an external field with horizontal and vertical components (h, v). Fluctuating two-valued variables (dipoles) are attached to the links of a two-dimensional square lattice, and the model is defined by assigning a set of Boltzmann weights (equivalently, interaction energies) to each allowed vertex configuration (see Fig. 1). The transfer matrix can be diagonalized exactly by the Bethe ansatz in its coordinate or algebraic version [7,8]. The phase diagram and the nature of the phase transitions are well understood when $h = v = 0$ (symmetric six-vertex), or when $h = 0$ and $v \neq 0$ [9,7]. If $h, v \neq 0$, some general features of the phase diagram have been described in [1] and the details of the calculation spelled out in [10], but a few questions have remained unanswered. The ferroelectric regime has been recently extensively reexamined [3,11] partly because of its connection to the 1D asymmetric diffusion problem [4]. In this regime, there exists also an equivalence between ferroelectric transitions at non-zero external field and a KPZ-type growth which, in its turn, is related to the equilibrium properties of facet–ridge endpoints on a BCC lattice [11,2–4].

In this paper we focus on the antiferroelectric regime where the free energy $f(h,v)$ remains constant as function of the field ('flat phase') in a bounded region of the (h,v) plane containing $h = v = 0$. This corresponds to the flat (001) crystal plane. Beyond this region, bounded by a curve Γ, the field is sufficiently strong to destroy the antiferroelectric order of the system, but not strong enough to impose ferroelectric order, and an incommensurate phase appears where the polarization (zero in the flat phase) changes continuously with the field. Here the spectrum of the transfer matrix is gapless with finite-size corrections typical of the gaussian model [12]. The singular part of the free energy, as Γ is approached from the incommensurate phase, has been partly determined. Lieb and Wu [7] calculated it along the $h=0$ line and found an exponent 3/2, later recognized as typical of a Pokrovskii–Talapov (PT) [13] phase transition [14]. By upgrading a result of Bogoliubov et al. [15], Kim has shown that finite-size corrections of the transfer matrix spectrum allow one to compute the Hessian of the free energy, which turns out to be related in a simple way to the gaussian coupling constant [12]. Still, the complete, exact form of the leading singular part of $f(h,v)$ near Γ has not been found. In this paper we study it near the two points on Γ, which we call (h_c,v_c) and $(-h_c,-v_c)$, where the tangent is parallel to the v-axis, and we find

$$
\begin{aligned}
f(h_c+\delta h, v_c) &= f(h_c,v_c) - \text{const}(\delta h)^{3/2}, \\
f(h_c, v_c+\delta v) &= f(h_c,v_c) - \text{const}|\delta v|^3 .
\end{aligned}
\tag{1.1}
$$

The two points are related by symmetry under arrow reversal, which implies $f(h,v) = f(-h,-v)$ [1], and the exponents in Eq. (1.1) measure the rounding off of the edges of the (001) facet.

Even though our calculation has been carried out only at these points of Γ, the technique we present should work in general, and our result, which generalizes Lieb and Wu's method and complements the finite-size techniques of Kim [12], strengthens the long held belief that the exponent 3/2 should govern the free energy singularity at every point of the phase boundary [2,3,10]. This exponent has been measured [16] in some experiments with Pb crystals some years ago. Our results however show that along the tangential direction 3/2 rescales to 3 and this fact, perhaps experimentally observable, holds presumably at any other point of Γ [17].

However, something more can be said about the nature of the phase transition along Γ.

The method of mapping a 2D statistical system into a 1D quantum spin chain has been fruitful and widely used in the past [18]. We pursue it here, regardless of the fact that the relevant spin chain, which turns out to be the asymmetric XXZ spin chain in a vertical field V, is not hermitian [19]. We find that the flat phase corresponds to a region in the (h,V) plane where the ground state energy does not depend on the fields and where excitations are massive. Along the transition line, analogue of Γ, the excitations become massless, but the point $(h_c, V = 0)$ (with its symmetric $(-h_c, V = 0)$) is singled out by the fact that dispersion relations obey the following law, at small momenta,

$$\Delta E \simeq (\Delta P)^{1/2}, \tag{1.2}$$

and finite-size corrections for low-lying excitations scale like

$$\Delta E \simeq N^{-1/2}, \tag{1.3}$$

where N is the length of the chain. At this point, analogue of (h_c, v_c) for the statistical model, the vanishing of the mass gap exhibits an exponent $1/2$ which does not appear at any other point of the transition line in the (h, V) plane. In Section 5 we propose an explanation of these results. Eqs. (1.2) and (1.3) are consistent with a PT transition viewed along the horizontal rather than the vertical direction. Yet, an argument based on the spectral decomposition of correlators shows that when (h_c, v_c) is reached from the commensurate phase, the vertical arrow correlation length diverges, while everywhere else along Γ the transition is induced by level crossing in the transfer matrix spectrum which prevents the divergence of the same correlation length. This points to the fact that (h_c, v_c) and $(-h_c, -v_c)$ are indeed different from all other points on Γ.

The paper is divided into five sections. In Section 2 we give definitions and summarize previously known results. In Section 3 hole excitations and the spectrum of the spin chain are studied and in Section 4 the method of Lieb and Wu is suitably extended to determine the free energy singularity when both h and v are non-zero. Section 5 contains an interpretation of the results.

2. Definitions

The model is a natural generalization of the well-known symmetric six-vertex model. Arrows are placed on the edges of an $N \times M$ square lattice and Boltzmann weights $R^{\beta\beta'}_{\alpha\alpha'}(u)$ are assigned to the vertices (see Fig. 1) so that the row-to-row transfer matrices

$$T(u)_{\{\underline{\alpha}\},\{\underline{\alpha}'\}} = \sum_{\{\underline{\beta}\}} \prod_{k=1}^{N} R^{\beta_k\beta_{k+1}}_{\alpha_k\alpha'_k}(u) \tag{2.1}$$

form a commuting family

$$[T(u), T(u')] = 0$$

for any two values u, u' of the spectral parameter [20]. The associated (integrable) spin chain,

$$\mathcal{H} = \sum_{j=1}^{N} \left[\frac{\cosh\gamma}{2}(1 + \sigma_j^z\sigma_{j+1}^z) - e^{2h}\sigma_j^+\sigma_{j+1}^- - e^{-2h}\sigma_j^-\sigma_{j+1}^+ \right] - V\sum_{j=1}^{N}\sigma_j^z, \tag{2.2}$$

is obtained from (2.1) by taking the so-called extremely anisotropic limit $(u \to 0)$

$$T(u) = \exp\left[(v+h)\sum_{j=1}^{N}\sigma_j^z\right]\overline{T}(u)\,,$$

$$\mathcal{H} = -V\frac{d}{dv}\log\left[\exp\left((v+h)\sum_{j=1}^{N}\sigma_j^z\right)\right] - \sinh\gamma\frac{d}{du}\log\overline{T}(u)|_{u=0}\,.$$

V breaks the $\mathbb{Z}_2$ symmetry of spin reversal while h breaks parity invariance (see Appendix A for a complete discussion of symmetries).

By means of the Bethe ansatz, eigenvalues of (2.1) and (2.2) are found from the solution of a set of coupled equations

$$\left[\frac{\sinh(\frac{\gamma}{2}+\frac{i\alpha_k}{2})}{\sinh(\frac{\gamma}{2}-\frac{i\alpha_k}{2})}\right]^N = (-1)^{n+1}e^{2hN}\prod_{l=1}^{n}\frac{\sinh(\gamma+\frac{i}{2}(\alpha_k-\alpha_l))}{\sinh(\gamma-\frac{i}{2}(\alpha_k-\alpha_l))}, \tag{2.3}$$
$$k=1,2,\dots,n$$

and given respectively by

$$\begin{aligned}\Lambda(u) &= e^{v(N-2n)}e^{hN}\left[\frac{\sinh(\gamma-u)}{\sinh\gamma}\right]^N\prod_{j=1}^{n}\frac{\sinh(\frac{\gamma}{2}+u-\frac{i\alpha_j}{2})}{\sinh(\frac{\gamma}{2}-u+\frac{i\alpha_j}{2})}\\ &\quad+e^{v(N-2n)}e^{-hN}\left[\frac{\sinh u}{\sinh\gamma}\right]^N\prod_{j=1}^{n}\frac{\sinh(\frac{-3\gamma}{2}+u-\frac{i\alpha_j}{2})}{\sinh(\frac{\gamma}{2}-u+\frac{i\alpha_j}{2})}\\ &= \Lambda_R(u)+\Lambda_L(u)\,,\end{aligned} \tag{2.4}$$

$$\begin{aligned}E &= N\cosh\gamma - \sum_{k=1}^{n}\frac{2\sinh^2\gamma}{\cosh\gamma-\cos\alpha_k} - V(N-2n)\\ &= N\cosh\gamma + \sum_{k=1}^{n}e(\alpha_k) - V(N-2n)\,.\end{aligned} \tag{2.5}$$

Here n stands for the number of reversed spins (arrows) with respect to the reference ferromagnetic state $|\uparrow\uparrow\dots\uparrow\rangle$. It is a conserved quantity since $S^z=\frac{1}{2}\sum_{j=1}^{N}\sigma_j^z$ commutes with $\mathcal{H}$ and $T(u)$.

Beside their energy, given by (2.5), the momentum can also be computed. $\overline{T}^{-1}(0)$ yields the right-shift operator $S=e^{-i\mathrm{P}}$,

$$S=|\alpha_1,\alpha_2,\dots,\alpha_M\rangle = |\alpha_\mathrm{M},\alpha_1,\alpha_2,\dots,\alpha_{M-1}\rangle\,, \tag{2.6}$$

and from (2.1) and (2.4) one gets

$$e^{-iP}=e^{-2hn}\prod_{j=1}^{n}\frac{\sinh(\frac{\gamma}{2}+\frac{i\alpha_j}{2})}{\sinh(\frac{\gamma}{2}-\frac{i\alpha_j}{2})}\,,\qquad P=-2inh-\sum_{j=1}^{n}p^0(\alpha_j) \tag{2.7}$$

with

$$p^0(\alpha) = -i\ln\left[\frac{\sinh(\frac{\gamma}{2}+\frac{i\alpha}{2})}{\sinh(\frac{\gamma}{2}-\frac{i\alpha}{2})}\right].$$

Unlike most integrable spin chains studied before, (2.2) is not hermitian for $h \neq 0$, even though the statistical model has physically sensible positive Boltzmann weights. The question arises whether (2.1) and (2.2) have a complete set of eigenvectors. By numerically diagonalizing the transfer matrix on small chains it appears that, even though a few eigenvalues are degenerate in some charge sectors, the eigenvectors are linearly independent. We will assume that a complete set of eigenvectors exists and it is given by the Bethe ansatz.

We first summarize, for the sake of completeness, some already known facts that have been published elsewhere, beginning with the spin chain because, although the Bethe-ansatz equations are identical, the form of the energy contribution from each rapidity α_k is simpler. Taking the logarithm of (2.3) in the usual way we get

$$p^0(\alpha_k) - \frac{1}{N}\sum_{l=1}^{n}\Theta(\alpha_k-\alpha_l) + 2ih = \frac{2\pi}{N}I_k, \quad k=1,2,\dots,n, \tag{2.8}$$

where I_k is half-odd (integer) if n is even (odd) and

$$\Theta(\alpha) = -i\ln\left[\frac{\sinh(\gamma+\frac{i\alpha}{2})}{\sinh(\gamma-\frac{i\alpha}{2})}\right].$$

We define $p^0(0) = \Theta(0) = 0$ and cuts are chosen to run from $i\gamma$ to $i\infty$ and from $-i\gamma$ to $-i\infty$ for $p^0(\alpha)$; from $2i\gamma$ to $i\infty$ and from $-2i\gamma$ to $-i\infty$ for $\Theta(\alpha)$. Notice from (2.3) that $\mathrm{Re}(\alpha) \in [-\pi,\pi]$ so $\mathrm{Re}(\alpha_k-\alpha_l) \in [-2\pi, 2\pi]$. The cuts are chosen so that $\Theta(\alpha)$ is analytical in $-2\gamma < \mathrm{Im}(\alpha) < 2\gamma$ and real, monotonically increasing when $\alpha \in [-2\pi, 2\pi]$. With these conventions, the ground state[4] at $h=0$ in each sector of fixed $S^z = \frac{N}{2} - n$ corresponds to a sequence of n consecutive numbers $\{I_k\}$ in (2.8), from $-(n-1)/2$ to $(n-1)/2$ symmetric around 0 [21]. The rapidities $\{\alpha_j\}$ are real and distributed symmetrically around $\alpha = 0$ too. As $h \neq 0$, the rapidities move into the complex plane along a curve C. In a standard way [10], one gets in the thermodynamic limit from (2.8)

$$p^0(\alpha) - \frac{1}{2\pi}\int_C d\beta\,\Theta(\alpha-\beta)R(\beta) + 2ih = 2\pi x, \quad -\frac{1-y}{4} \leqslant x \leqslant \frac{1-y}{4}, \tag{2.9}$$

x is the real parameter of the curve, y is the polarization defined through

$$y = \lim_{N\to\infty}\frac{2S^z}{N} = \lim_{N\to\infty}\left(1-\frac{2n}{N}\right) \tag{2.10}$$

and the rapidity density $R(\alpha_l) = \lim_{N\to\infty} 2\pi/N(\alpha_{l+1}-\alpha_l)$ is determined by solving the integral equation

[4] When (2,2) is not hermitean, by ground state we mean the state whose eigenvalue has the lowest real part.

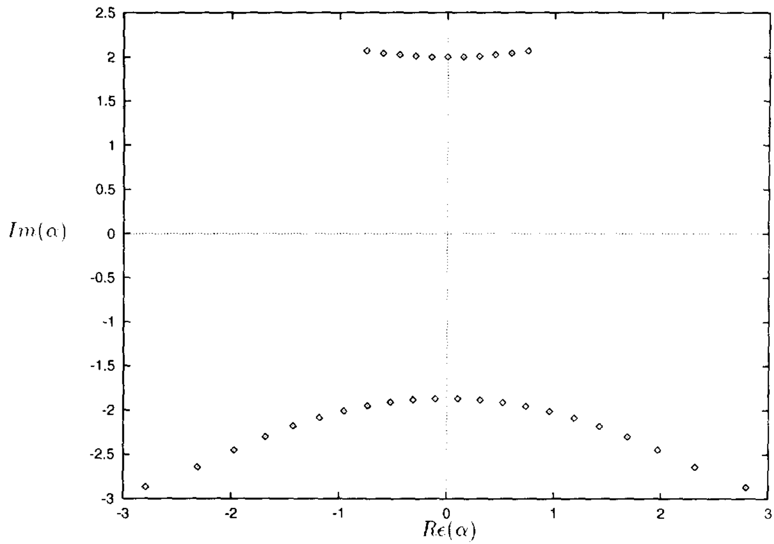

Fig. 2. Distribution of the rapidities α_k for $N = 44$. The lower curve corresponds to the ground state in the sector with $n = N/2$ and $\exp(2h) = 9$, the upper curve to the ground state of the sector with $n = N/4$ and $\exp(2h) = 1/9$.

$$\xi(\alpha) - \frac{1}{2\pi}\int_C d\beta\, K(\alpha-\beta)R(\beta) = R(\alpha)\,, \tag{2.11}$$

where

$$\xi(\alpha) = \frac{dp^0(\alpha)}{d\alpha}\,, \qquad K(\alpha) = \frac{d\Theta(\alpha)}{d\alpha}\,.$$

The energy and the polarization are thus given by

$$\lim_{N\to\infty}\frac{E}{N} = \cosh\gamma + \frac{1}{2\pi}\int_C d\alpha\, e(\alpha)R(\alpha) - Vy\,, \tag{2.12}$$

$$\frac{1-y}{2} = \frac{1}{2\pi}\int_C d\alpha\, R(\alpha)\,. \tag{2.13}$$

Some preliminary information about the shape of C and its location in the complex plane can be obtained by solving (2.3) numerically. We take as initial solution that composed of real roots and corresponding to the ground state, at fixed S^z, for $h = 0$. By the Perron–Frobenius theorem [21,22], the relevant eigenstate remains the ground state at fixed S^z even when $h \neq 0$, and the eigenvalue is real. It appears that for $h > 0$ ($h < 0$) the rapidities move into the lower (upper) half-plane as shown in Fig. 2.

The curve C is invariant under $\alpha \to -\alpha^*$, which is to be expected, this transformation being a symmetry of (2.3), so we will set $A = -a+ib$ and $B = a+ib$ to be the endpoints of the curve. Note that this property makes E real, as it should.

Strictly speaking $R(\alpha)$ is defined on C only, but (2.11) can be used to define it outside of C. If C is contained in the strip $-\gamma < \mathrm{Im}(\alpha) < \gamma$, $R(\alpha)$ is analytic in $-\gamma < \mathrm{Im}(\alpha) < \gamma$, but it inherits the poles of $\xi(\alpha)$ at $\pm i\gamma$. Let us consider the curve for which $a = \pi$. In this case, since $R(\alpha)$ is 2π periodic, (2.11) can be solved straightforwardly by Fourier transform. The solution is

$$R(\alpha) = \sum_n \frac{e^{-in\alpha}}{2\cosh\gamma n}, \quad -\gamma < \mathrm{Im}(\alpha) < \gamma. \tag{2.14}$$

Here and in the following, sums are understood to run from $-\infty$ to ∞ unless otherwise stated. Beyond this strip (2.14) can be expressed using elliptic functions. Introducing the complete elliptic integrals of the first kind I (I') of modulus k (k'), with $k^2+k'^2 = 1$ [23], related to γ by

$$\frac{I'(k)}{I(k)} = \frac{\gamma}{\pi},$$

the solution of (2.11) in a wider domain reads [24,23]

$$R(\alpha) = \frac{I(k)}{\pi}\mathrm{dn}\left(\frac{I(k)\alpha}{\pi}; k\right). \tag{2.15}$$

Notice the presence of a pole at $\alpha = \pm i\gamma$, inherited from $\xi(\alpha)$, which prevents the convergence of (2.14) beyond the smaller domain. The energy remains constant at its value for $h = 0$

$$e_0 = \lim_{N\to\infty} \frac{E_0}{N} = \cosh\gamma - 2\sinh\gamma \sum_n \frac{e^{-\gamma|n|}}{2\cosh\gamma n}$$

and from (2.13) $y = 0$. In fact the solution considered here has $n = N/2$ rapidities ($S^z = 0$) and, as it will be shown in the next section, E_0 is the ground state energy for h and V sufficiently close to 0.

As to the precise position of the curve, one has to revert to (2.9). Since $\Theta(\alpha+2\pi) = \Theta(\alpha) + 2\pi$, we use the expansion

$$\Theta(\alpha) = \alpha + i\sum_{n\neq 0} \frac{e^{-in\alpha-2\gamma|n|}}{n}, \quad -2\gamma < \mathrm{Im}(\alpha) < 2\gamma$$

and

$$p^0(\alpha) = \alpha + i\sum_{n\neq 0} \frac{e^{-in\alpha-\gamma|n|}}{n}, \tag{2.16}$$

and we introduce

$$p(\alpha) = \frac{\alpha}{2} + i\sum_{n\neq 0} \frac{e^{-in\alpha}}{2n\cosh\gamma n} = \mathrm{am}\left(\frac{I(k)\alpha}{\pi}; k\right). \tag{2.17}$$

The series in (2.16) and (2.17) are certainly convergent when $-\gamma < \mathrm{Im}(\alpha) < \gamma$, but they converge also at $\alpha = \pm\pi \pm i\gamma$, because of the alternating sign. Eq. (2.9) reduces to

$$p(\alpha) + \frac{ib}{2} + i\sum_{n\neq 0}(-)^n \frac{e^{nb}}{2n\cosh\gamma n} + 2ih = 2\pi x\,, \quad -\frac{1}{4} \leqslant x \leqslant \frac{1}{4}\,.$$

Specialization to the endpoints permits relating the value of h to b [7,10]

$$h(b) = -\frac{b}{2} - \sum_{n=1}^{\infty}(-)^n \frac{\sinh nb}{n\cosh n\gamma} \tag{2.18}$$

so that the final equation of the curve is

$$p(\alpha) + ih = 2\pi x\,, \quad -\frac{1}{4} \leqslant x \leqslant \frac{1}{4}\,.$$

Notice that the points on the curve are characterized by

$$\mathrm{Im}(p(\alpha)) + h = 0\,. \tag{2.19}$$

We set $h_c = h(b = -\gamma)$. One might suspect that, when $h > h_c$, the endpoints would remain at $a = \pi$ but with $b < -\gamma$ (or $b > \gamma$ if $h < -h_c$). If C does not cross the point $-i\gamma$, where $\xi(\alpha)$ has a pole, it can always be deformed to the real axis in (2.11)

$$R(\alpha) + \frac{1}{2\pi}\int_{-\pi}^{\pi} du\, K(\alpha - u)R(u) = \xi(\alpha) \tag{2.20}$$

so that the solution is still given by

$$\frac{I(k)}{\pi}\mathrm{dn}\left(\frac{I(k)}{\pi}\alpha; k\right),$$

but the expansion (2.14) is no longer useful. To find the $h(b)$ relation, we close C in (2.9) to the real axis, and take $\alpha = A$,

$$p^0(A) - \frac{1}{2\pi}\int_{-\pi}^{\pi} du\, \Theta(A - u)R(u) + \int_{-\pi}^{A} d\beta\, R(\beta) + 2ih = -\frac{\pi}{2}\,. \tag{2.21}$$

The integral of $R(\alpha)$ is obtained by integrating both sides of (2.20), and from (2.21) we conclude

$$2h(b) = b + 2\ln\frac{\cosh\left(\frac{\gamma}{2} - \frac{b}{2}\right)}{\cosh\left(\frac{\gamma}{2} + \frac{b}{2}\right)} + 2\sum_{n>0}(-)^n \frac{e^{-2n\gamma}\sinh nb}{n\cosh n\gamma}\,, \tag{2.22}$$

which reduces to (2.18) when $|b| \leqslant \gamma$. Eq. (2.22) though cannot give the right dependence $h(b)$ at $|b| > \gamma$, because $h(b)$ decreases when $b < -\gamma$ and increases for $b > \gamma$, going back to the range of values it had as $b \in [-\gamma, \gamma]$. Clearly the initial assumption $a = \pi$ cannot be correct. To gain more insight we resort as usual to the numerical solution of (2.3), which shows that, as $h > h_c$, the curve with $y = 0$ has

Table 1
Position of the endpoints $\pm a + ib$ of the curve C for $h < h_c$; $\exp(2h) = 3$

Lattice size	a	b
8	2.226901585	−1.186380535
12	2.522418777	−1.215745628
16	2.674453171	−1.227403536
20	2.766810718	−1.233071106
24	2.828778340	−1.236225697
28	2.873206253	−1.238154458
32	2.906605731	−1.239417236
36	2.932624180	−1.240288031
40	2.953462078	−1.240913442
Extrap. ∞	3.141592659(9)	−1.243603723(1)
	$\pi = 3.141592653$	$-\gamma = -3.737102242$

Table 2
Position of the endpoints $\pm a + ib$ of the curve C for $h > h_c$; $\exp(2h) = 18$

Lattice size	a	b
8	1.345603261	−3.0497549071
12	1.479730321	−3.2366686985
16	1.535932819	−3.3472122872
20	1.564274277	−3.4190538006
24	1.580405494	−3.4690826450
28	1.590409443	−3.5057653322
32	1.597021761	−3.5337453681
36	1.601612009	−3.5557588049
40	1.604924714	−3.5735136386
Extrap. ∞	1.6193362(3)	−3.737102232(7)
	$\pi = 3.141592653$	$-\gamma = -3.737102242$

endpoints at (see Table 2. For comparison with the case $h < h_c$ see Table 1. Note that all extrapolations presented in the tables have been done using data up to 80 sites. We give however only the first values, up to $N = 40$, for they already show clearly that the values are converging towards a limit. All tables have been calculated for $\cosh\gamma = 21$, where $\exp(2h_c) = 10.51787$)

$$b = -\gamma, \qquad a < \pi.$$

This (new) result will be used in the calculation of the free energy singularity in Section 4.

Turning next to the statistical model, the largest eigenvalue of the transfer matrix yields the free energy per site (we drop here the inessential factor β)

$$f(u,\gamma,h,v) = -\lim_{N\to\infty} \frac{\ln \Lambda_0(u,\gamma,h,v)}{N}$$

whose value, as $N \to \infty$, is dominated by the largest of the two limits

$$\lim_{N\to\infty}\frac{1}{N}\ln \Lambda_{\rm R}(u) = F_{\rm R}(u,\gamma,h,y)+vy = h+\ln\frac{\sinh(\gamma-u)}{\sinh\gamma}+vy + \frac{1}{2\pi}\int_C d\alpha\, R(\alpha) f_{\rm R}(\alpha;u)\,,$$

$$\lim_{N\to\infty}\frac{1}{N}\ln \Lambda_{\rm L}(u) = F_{\rm L}(u,\gamma,h,y)+vy = -h+\ln\frac{\sinh(u)}{\sinh\gamma}+vy + \frac{1}{2\pi}\int_C d\alpha\, R(\alpha) f_{\rm L}(\alpha;u)\,,$$

where we have defined

$$f_{\rm R}(\alpha;u) = \ln\frac{\sinh(\frac{\gamma}{2}+u-\frac{i\alpha_j}{2})}{\sinh(\frac{\gamma}{2}-u+\frac{i\alpha_j}{2})}\,,$$

$$f_{\rm L}(\alpha;u) = \ln\frac{\sinh(\frac{-3\gamma}{2}+u-\frac{i\alpha_j}{2})}{\sinh(\frac{\gamma}{2}-u+\frac{i\alpha_j}{2})}\,.$$

If $F_{\rm R}$, $F_{\rm L}$ are known, and we call F the dominant one, the equilibrium value of y and the free energy are determined by the minimum condition

$$f(u,\gamma,h,v) = \min_{-1\leqslant y\leqslant 1}\{-F(u,\gamma,h,y)-vy\}\,. \tag{2.23}$$

When $-h_c \leqslant h \leqslant h_c$ and for small enough values of v, the state defined by C ($a=\pi$; $-\gamma\leqslant b\leqslant\gamma$) also yields the largest eigenvalue of the transfer matrix. The free energy [5]

$$f(u,\gamma,h,v) = -2\sum_{n=1}^{\infty}\frac{e^{-2\gamma n}}{n\cosh\gamma n}\sinh(nu)\sinh n(\gamma-u) \tag{2.24}$$

is constant in a whole region of the (h,v) plane bounded by a curve Γ ('flat' phase). The parametric equation $(h(b),v(b))$ of Γ is given by (2.20) and by

$$v(b) = -\left.\frac{\partial F}{\partial y}\right|_{h\ \text{fixed},\, y=0}$$

which can be explicitly computed

$$2v(b) = \gamma-|\gamma-2u-b|+2\sum_{n=1}^{\infty}\frac{(-)^n}{n}\frac{\sinh[n(\gamma-|\gamma-2u-b|)]}{\cosh n\gamma}\,, \tag{2.25}$$

$$-\gamma\leqslant b\leqslant\gamma\,.$$

The other half of the curve Γ (see Fig. 3) can be recovered from the symmetry $f(-h,-v) = f(h,v)$ (see Appendix A). Most of these results have been obtained

[5] The only part in which our analysis differs from Ref. [10] is that $\Lambda_{\rm R}$ is exponentially larger for $d<\gamma-2u$ and $\Lambda_{\rm L}$ for $d>\gamma-2u$, where id is the point in which C crosses the imaginary axis. A comparison of (2.24) with Ref. [10] should take into account the different normalization of the Boltzmann weights.

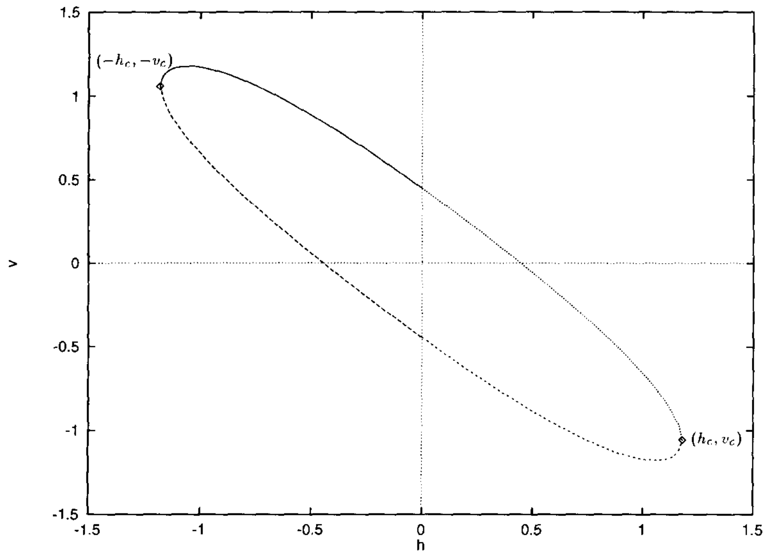

Fig. 3. Curve Γ in the h-v plane for $u = \frac{1}{2}$ and $\cosh(\gamma) = 21$.

elsewhere and we have presented them here only for the sake of completeness. It should be pointed out that the fact that the ground state energy does not depend on h is simply a consequence of the analogous property of the free energy.

3. Hole excitations of the spin chain

To understand the nature of the phase transition along Γ we turn to the calculation of the excitation energies, and we set $V = 0$, since the role of V is simply to shift the spectra at $S^z \neq 0$. As proven in Appendix A it is sufficient to consider $h \geqslant 0$.

A complete treatment of the spectrum should rely on the classification of all possible solutions of (2.3). This is usually done in the framework of the string hypothesis, according to which complex rapidities (at $h = 0$) have an imaginary part which tends to well-defined values in the thermodynamic limit. Exceptional solutions other than strings, but that still appear in complex conjugate pairs, can be handled in a similar way [25]. Yet, from the numerical analysis of (2.3), it appears that strings do not survive at moderately strong values of h. Therefore, we shall limit our calculation to the so-called hole excitations, that is holes in the ground state distribution of rapidities, occurring in sectors with $S^z > 0$ ($n < n_0 = N/2$). We introduce the counting function

$$Z(\alpha, \{\alpha_j\}) = \frac{p^0(\alpha)}{2\pi} - \frac{1}{2\pi N}\sum_{j=1}^{n} \Theta(\alpha - \alpha_j) + i\frac{h}{\pi} \tag{3.1}$$

so that (2.8) is rewritten

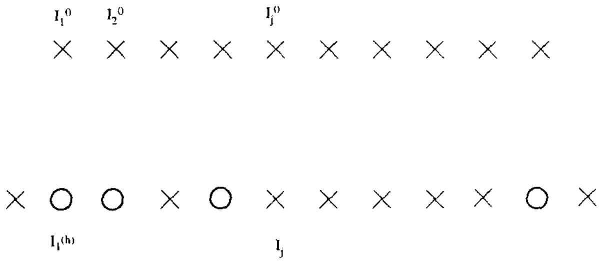

Fig. 4. Distribution of I_k's for the ground state and an excited state with $n = n_0 - 2$ rapidities.

$$Z(\alpha_k) = \frac{I_k}{N}.$$

Set vac = number of vacancies available for the quantum numbers $\{I_k\}$. With the usual hypothesis that $Z(\alpha)$ be monotonically increasing, we have

$$\Delta Z \stackrel{\text{def}}{=} Z(\alpha)|_{\text{Re}(\alpha)=\pi} - Z(\alpha)|_{\text{Re}(\alpha)=-\pi} = \frac{\text{vac}}{\text{N}}. \tag{3.2}$$

On the other hand, from (3.1), we find $\Delta Z = 1 - (n/N)$. For the ground state $n = n_0 = N/2$ and so vac $= n_0$, i.e. the available vacancies are all filled. For n rapidities, $n = n_0 - r$, where $r = 1, 2, \ldots$, we have

$$\Delta Z = 1 - \frac{n_0 - r}{N}, \qquad \text{vac} = n_0 + r$$

so that $n_0 + r$ vacancies are partially filled with $(n_0 - r)$ I_k's, leaving $N_h = 2r$ holes.

We will resort to the 'backflow method' [24,26] in dealing with (2.5), (3.1) and (2.7) in the limit $N \to \infty$. The calculation differs slightly for the 2 cases r = even or odd, but the results are identical and we will present the case r = even only. If this is the case, then $n = n_0 \pmod 2$ and the quantum numbers $\{I_k\}$ of the excited state have the same oddness of the quantum numbers $\{I_k^0\}$ of the ground state. We assume that the r additional vacancies for $\{I_k\}$ are placed $r/2$ to the left and $r/2$ to the right of the sequence (see Fig. 4).

We call $\{\beta_j^{(1)}\}$ the $r/2$ additional rapidities at the left edge, $\{\beta_j^{(2)}\}$ the $r/2$ additional rapidities at the right edge and $\{\alpha_j^{(h)}\}$ the N_h holes. Then, for the ground state

$$Z_0(\alpha) = \frac{p^0(\alpha)}{2\pi} - \frac{1}{2\pi N}\sum_{j=1}^{n_0} \Theta(\alpha - \alpha_j^0) + i\frac{h}{\pi}, \tag{3.3}$$

$$Z_0(\alpha_k^0) = \frac{I_k^0}{N}, \tag{3.4}$$

and for the excited state, adding and subtracting the holes

$$Z(\alpha) = \frac{p^0(\alpha)}{2\pi} - \frac{1}{2\pi N}\sum_{j=1}^{n_0} \Theta(\alpha - \alpha_j) + \frac{1}{2\pi N}\sum_{j=1}^{N_h} \Theta(\alpha - \alpha_j^{(h)})$$

$$-\frac{1}{2\pi N}\sum_{j=1}^{r/2}\left[\Theta(\alpha-\beta_j^{(1)})+\Theta(\alpha-\beta_j^{(2)})\right]+i\frac{h}{\pi}, \tag{3.5}$$

$$Z(\alpha_k)=\frac{I_k}{N}, \qquad Z(\alpha_j^{(h)})=\frac{I_j^{(h)}}{N}. \tag{3.6}$$

As $N\to\infty$ $\{\beta_j^{(1)}\}\to A$ and $\{\beta_j^{(2)}\}\to B$. Subtracting (3.4) from (3.6) and retaining terms of order $1/N$ (this is a standard Bethe-ansatz calculation) [26] we find that

$$j(\alpha_l)=\lim_{N\to\infty}\frac{\alpha_l-\alpha_l^0}{\alpha_{l+1}^0-\alpha_l^0}$$

satisfies

$$j(\alpha)+\frac{1}{2\pi}\int_C d\beta\, K(\alpha-\beta)j(\beta)=-\frac{1}{2\pi}\sum_{j=1}^{N_h}\Theta(\alpha-\alpha_j^{(h)})$$
$$+\frac{r}{4\pi}\left[\Theta(\alpha-B)+\Theta(\alpha-A)\right] \tag{3.7}$$

with

$$\Delta E=\int_C d\alpha\, e'(\alpha)j(\alpha)-\sum_{j=1}^{N_h}e(\alpha_j^{(h)})+\frac{r}{2}\left(e(A)+e(B)\right),$$

$$\Delta P=ihN_h-\int_C d\alpha\,\xi(\alpha)j(\alpha)+\sum_{j=1}^{N_h}p^0(\alpha_j^{(h)})-\frac{r}{2}\left(p^0(A)+p^0(B)\right).$$

Eq. (3.7) defines the analytical properties of $j(\alpha)$ in the complex plane. Since for $0\leqslant h\leqslant h_c$ the curve C is contained in $-\gamma\leqslant \mathrm{Im}(\alpha)\leqslant 0$, $j(\alpha)$ is certainly analytic in $-2\gamma<\mathrm{Im}(\alpha)<\gamma$ and the curve can be closed to the real axis. Noticing, from (3.7), that $j(\alpha+2\pi)-j(\alpha)=-N_h/2$ we get, with $u\in[-\pi,\pi]$,

$$j(u)+\frac{1}{2\pi}\int_{-\pi}^{\pi}dv\, K(u-v)j(v)=\frac{N_h}{4\pi}\Theta(u+\pi)-\frac{1}{2\pi}\sum_{j=1}^{N_h}\Theta(u-\alpha_j^{(h)})-\frac{r}{2}, \tag{3.8}$$

$$\Delta E=\int_{-\pi}^{\pi}du\, e'(u)j(u)+\frac{N_h}{2}e(\pi)-\sum_{j=1}^{N_h}e(\alpha_j^{(h)}), \tag{3.9}$$

$$\Delta P=ihN_h-\int_{-\pi}^{\pi}du\,\xi(u)j(u)+\sum_{j=1}^{N_h}p^0(\alpha_j^{(h)}). \tag{3.10}$$

Eq. (3.8) can be solved by Fourier transform, paying attention to the fact that $j(u)$ is not periodic, but obeys the quasiperiodicity condition $j(u+2\pi)-j(u)=-N_h/2$. Alternatively, and with identical results, the symmetric integral operator $(\mathbf{1}+\frac{1}{2\pi}\mathbf{K})$ at the left side of (3.8) can be formally inverted and the solution plugged in (3.9) and (3.10) [26]. The result has the usual additive form

$$\Delta E = 2\sinh\gamma \sum_{j=1}^{N_h} \epsilon(\alpha_j^{(h)}), \tag{3.11}$$

where the dressed energy $\epsilon(u)$ satisfies

$$\epsilon(u) + \frac{1}{2\pi}\int_{-\pi}^{\pi} dv\, K(u-v)\epsilon(v) = \xi(u)$$

and therefore coincides with $R(u) = \frac{I(k)}{\pi}\,\mathrm{dn}\left(\frac{I(k)u}{\pi};k\right)$. As to the momentum, one has

$$\Delta P = \sum_{j=1}^{N_h}\left[p(\alpha_j^{(h)}) + ih\right], \tag{3.12}$$

where $p(\alpha)$ has been defined in (2.17). The calculation for r odd differs slightly in the intermediate steps but also yields (3.11) and (3.12), which are then true for N_h arbitrary (but obviously even). The fact that N_h is even was missed in [27] where, following the same assumption made in [24], one hole was kept fixed at the edge. In other words, only a subset of the two-hole band of states was dealt with. [6]

Eqs. (3.11) and (3.12) are simple generalizations of their limit at $h = 0$, since h appears only additively in ΔP and, implicitly, in the position of the hole which is bound to be on the curve C. This simple dependence could not be derived immediately from (2.5) and (2.7) because the rapidities $\{\alpha\}$ depend on h in a non-trivial way through (2.3), and only the explicit calculation guarantees that (3.11) and (3.12) are correct.

Several comments are in order. Unlike the energy, which being the eigenvalue of a non-hermitian operator can, and indeed does have an imaginary part, the momentum must be real. This is guaranteed by (2.19), since $\alpha^{(h)} \in \mathbb{C}$. It is well known that, from (2.7), (2.8) and the oddness of $\Theta(\alpha)$, the momentum can be obtained by summing (2.8) over k,

$$P = -\frac{2\pi}{N}\sum_{k=1}^{n} I_k. \tag{3.13}$$

The momentum of the ground state P^0 is therefore always zero, while the momentum of an excited state is

$$P = \frac{2\pi}{N}\sum_{k=1}^{N_h} I_k^{(h)}$$

from which one sees that, as $N \to \infty$, $-\frac{\pi}{2} \leqslant \Delta P(\text{hole}) \leqslant \frac{\pi}{2}$. This is also confirmed by (2.17) and (3.12). The dispersion relations are obtained by eliminating $\alpha^{(h)}$ in (3.11) and (3.12) using

[6] One of the authors (G.A.) is grateful to Prof. C. Destri for pointing this out.

Table 3
Energy gap of the spin chain for the first excited state for different values of h compared to the analytical result (3.15)

Lattice size	$e^{2h} = 1.0$	$e^{2h} = 9.0$
8	38.8549946261240	27.3592680025296
12	38.4729554492734	23.5353424072427
16	38.3095545699746	21.4216001709441
20	38.2251709688714	20.0937869680560
24	38.1760618666305	19.1948069770300
28	38.1450125441243	18.5549980007490
32	38.1241500821837	18.0828136699350
36	38.1094640015976	17.7244227601235
40	38.0987382252780	17.4461598430727
Extrap. ∞	38.04991359(1)	15.8884(8)
Exact eq.	38.04991361	15.8887254

$$\mathrm{dn}(\alpha; k) = \sqrt{1 - k^2 \sin^2(\mathrm{am}(\alpha; k))}\,,$$

which yields

$$\Delta E(\Delta P) = m_0\sqrt{1 - k^2 \sin^2(\Delta P - ih)}\,, \qquad m_0 = 2\sinh\gamma\frac{I(k)}{\pi}\,. \tag{3.14}$$

An apparent discrepancy with Gaudin's result (for the case $h = 0$) is clarified in Appendix B. The $\mathrm{dn}(\alpha)$ function (and consequently $\epsilon(\alpha)$) has a non-negative real part in the rectangle $[-\pi; -\pi - i\gamma; \pi - i\gamma; \pi]$ and this lifts the ambiguity in the sign of (3.14). It also confirms that the choice of the ground state was correct, because the real part of the energy, at least under 'small' variations (a countable number of holes), increases. The minimum of $\mathrm{Re}(\Delta E)$ is reached when $\alpha^{(h)} = A$ or B. When this happens $\Delta P = \pm\frac{\pi}{2}$ and the gap in the spectrum is (remember that 2 holes are present in the lowest excited state)

$$\Delta E(\mathrm{gap}) = 2m_0\sqrt{1 - k^2\cosh^2(h)}\,, \tag{3.15}$$

which guarantees that the 'mass gap' is real (see Table 3 for a comparison with numerical results). In particular it vanishes at $b = -\gamma$, that is when $A = -\pi - i\gamma$, $B = \pi - i\gamma$ and

$$h = h_c = \frac{\gamma}{2} + \sum_{n\neq 0}(-)^n \frac{\sinh(n\gamma)}{n\cosh(n\gamma)}\,.$$

This is most easily seen from (3.11)

$$\Delta E(\mathrm{gap}) = 2m_0\,\mathrm{dn}\left(\frac{I(k)}{\pi}(\pm\pi - i\gamma); k\right) = 2m_0\,\mathrm{dn}(\pm I(k) - iI'(k); k) = 0\,.$$

Therefore, from (3.15) an alternative equation for h_c is

$$\cosh(h_c) = \frac{1}{k}\,.$$

It is particularly interesting to see how the mass gap vanishes as $h \to h_c$

$$\Delta E(\text{gap}) \sim 2^{3/2} m_0 \sqrt{k'} (h_c - h)^{1/2} + O(h_c - h) . \quad (3.16)$$

The vanishing with an exponent 1/2 is peculiar of the point under consideration, as it will appear clear from the general case, to be discussed later, which includes the vertical field V. Finally, we specialize (3.15) at $h = h_c$. Then the hole excitations are massless and if we set $\Delta P = -\frac{\pi}{2} + \epsilon$ or $\Delta P = \frac{\pi}{2} - \epsilon$, $0 < \epsilon \ll 1$, we get, respectively

$$\Delta E(\Delta P) \sim 2m_0 \sqrt{\mp 2ik'}\, \epsilon^{1/2} . \quad (3.17)$$

This dispersion relation is certainly surprising and reflects itself in the peculiar behavior of the finite-size corrections of the low-lying energy gaps at $h = h_c$. In marked contrast with the $\mathcal{O}(\frac{1}{N})$ scaling typical of spin chains, which describe conformally invariant models in the continuum limit [28], we find

$$\Delta E \sim \frac{c}{N^{1/2}} + O(N^{-1}) , \quad (3.18)$$

where c depends on the state under consideration. The momentum being quantized in units of $2\pi/N$ on the finite lattice (3.13), this behavior is well in agreement with (3.17).

The sector $S^z = 0$ deserves a special comment. Not knowing what takes the place of strings, the analysis of the excitations has been necessarily numerical. Two things have been determined. Setting $E_0(S^z = 0, N, h)$ and $E_1(S^z = 0, N, h)$ to be respectively the ground state and the lowest lying of the first band of excited states in the sector $S^z = 0$, on a chain of N sites, and at fixed horizontal field $h \leqslant h_c$, we found

$$\Delta E(S^z = 0, h) = \lim_{N \to \infty} \left[E_1(S^z = 0, N, h) - E_0(S^z = 0, N, h) \right] \quad (3.19)$$

to be positive, non-zero for $h < h_c$ and

$$\lim_{h \to h_c^-} \Delta E(S^z = 0, h) = 0$$

so that, even in this sector, the spectrum becomes massless at $h = h_c$ (see Table 4). Secondly, the $\mathcal{O}(N^{-1/2})$ scaling is preserved at h_c (see Table 5)

$$E_1(S^z = 0, N, h_c) - E_0(S^z = 0, N, h_c) \sim \frac{c}{N^{1/2}} , \quad N \gg 1 .$$

E_1 must not be confused with the other (degenerate in the thermodynamic limit) ground state that appears in this sector at momentum $P = \pi$ and is responsible for the spontaneous breaking of the arrow-reversal symmetry in the symmetric six-vertex model [9,24]. Since we do not study the order parameter (staggered polarization) this state will not be discussed here.

We can now reintroduce V, whose effect is to shift the spectra at $S^z \neq 0$. The mass gap for a state with $n = n_0 \pm r$, and consequently $2r$ holes is easily read from (2.5) and (3.15)

$$\Delta E(\text{gap}; n) = 2rm_0 \sqrt{1 - k^2 \cosh^2(h)} - 2V(\pm r) . \quad (3.20)$$

Table 4
Mass gap of the spin chain in the sector $S^z = 0$ for different values of $h \leqslant h_c$

Lattice size	$e^{2h} = 9.0$	$e^{2h} = 9.5$	$e^{2h} = 10.0$	$e^{2h_c} = 10.51787$
8	40.28463586426577	40.60665243638542	41.00560893816288	41.50186071099847
12	32.50806556257382	32.33242547913501	32.27369006467646	32.34509918439876
16	28.03119022066448	27.47527007849106	27.06291429820305	26.80804074773090
20	25.23278497081201	24.37422080701744	23.67516261790179	23.15771126310622
24	23.35422673956813	22.24638140499817	21.30438602193786	20.56522041772249
28	22.02474072486461	20.70732422258583	19.55338243467817	18.62033939778466
32	21.04552971555199	19.54981005828927	18.20747202515815	17.10061549106331
36	20.30141022559842	18.65287555243093	17.14104807658379	15.87553491911761
40	19.72145517781357	17.94130164070793	16.27579201027032	14.86352304583235
Extrap. ∞	15.946(3)	13.054(9)	9.37499(4)	$-1.3(3) \times 10^{-5}$

Table 5
Exponent of N for the finite-size corrections of the energy gap in the sector $S^z = 0$ on the critical line $h = h_c$

Lattice size	Exponent
8	−0.6147896371667922
12	−0.6526671750014708
16	−0.6559635919155932
20	−0.6511929107450443
24	−0.6444786397317260
28	−0.6376031966136601
32	−0.6311198906745727
36	−0.6251786621408798
40	−0.6197881465618827
Extrap. ∞	−0.5031(1)
Expected value	−0.5

An alternative way to reach the boundary with the massless phase is to have a sufficiently large $|V|$. From (3.20) the crossing occurs at

$$V = \pm m_0 \sqrt{1 - k^2 \cosh^2(h)} \tag{3.21}$$

and moves the ground state to sectors of $S^z > 0$ (i.e. $n < n_0$) if $V > 0$, and to sectors of $S^z < 0$ (i.e. $n > n_0$) if $V < 0$, as it was intuitively predictable from (2.5). Notice that, unlike what happens in (3.16), the mass gap goes to zero linearly in V or linearly in h if $V \neq 0$ were kept fixed and $h \to h(V)$, where $h(V)$ is defined by (3.21). The point $V = 0$, $h = h_c$ (or equivalently $h = -h_c$), where the exponent 1/2 of (3.16) appears, is clearly special. Even if it were approached by changing h and V simultaneously, the term $(h_c - h)^{1/2}$ would dominate over the linear term in V. There is no way to erase this effect because it is impossible to reach $(h_c, V = 0)$ by changing V only: the line $h = h_c$ in the (h, V) plane is tangent to the phase boundary curve defined by (3.21).

This result may look odd, because the energy difference between sectors of different S^z corresponds to the step free energy for the statistical model, and from (2.4) it is hard to see how it could vanish other than linearly. Yet it is readily seen that the phenomenon is not an artifact of the spin chain. An explicit calculation of the step free energy

$$f_{\rm step} = -\left[\ln \Lambda_{\max}(S^z = 1) - \ln \Lambda_{\max}(S^z = 0)\right]$$

can be by-passed observing that the vanishing of $f_{\rm step}$ signals the transition to the incommensurate phase and therefore must be given by (2.25)

$$f_{\rm step} = 2v - \gamma + |\gamma - 2u - b| - 2\sum_{n=1}^{\infty} \frac{(-)^n}{n} \frac{\sinh[n(\gamma - |\gamma - 2u - b|)]}{\cosh n\gamma},$$

$$-\gamma \leqslant b \leqslant \gamma .$$

The points (h_c, v_c) and $(-h_c, -v_c)$, reached on Γ when $b = -\gamma$ (or γ) are the equivalent of $(\pm h_c, V = 0)$ in the spin-chain phase diagram. They, again, cannot be approached from the flat phase by changing v only, since the line $h = h_c$ in the (h, v) plane is tangent to Γ. But, from (2.18), near $b = -\gamma$,

$$h_c - h \sim \frac{1}{2}\left(\frac{I(k)}{\pi}\right)^2 k'(b + \gamma)^2$$

and since $f_{\rm step}$ is linear in b near $b = -\gamma$ (unless $u = 0$)

$$f_{\rm step} \sim {\rm const}\,(h_c - h)^{1/2} + {\rm const}\,(v - v_c)$$

at (h_c, v_c). This shows that, like for the spin chain, the exponent 1/2 dominates and signals that the points (h_c, v_c) and $(-h_c, -v_c)$ are essentially different from the other points of Γ.

As to the sector $S^z = 0$, we have to extend the numerical analysis carried out for the spin chain. If $\Lambda_0(S^z = 0, N, h, v_c)$ and $\Lambda_1(S^z = 0, N, h, v_c)$ are the largest and next-to-largest eigenvalues on the finite lattice in the sector under consideration, we find that

$$\Delta \ln \Lambda(S^z = 0, h, v_c) = -\lim_{N\to\infty}\left[\ln \Lambda_1(S^z = 0, N, h, v_c) - \ln \Lambda_0(S^z = 0, N, h, v_c)\right]$$

is positive for $h < h_c$ and vanishes when $h = h_c$. Furthermore,

$$-\left[\ln \Lambda_1(S^z = 0, N, h_c, v_c) - \ln \Lambda_0(S^z = 0, N, h_c, v_c)\right] \sim \frac{c'}{N^{1/2}}, \qquad N \gg 1$$

in perfect correspondence with the spin-chain scaling of low-lying excitations (see Table 6).

4. The exponent 3/2 of the free energy singularity

As the field crosses the critical value of the Γ line (2.18), (2.25) the system enters a phase where horizontal and vertical polarizations, zero in the "flat phase", start to change

Table 6
Exponent for the scaling of the free energy gap in the sector $S^z = 0$

Lattice size	Exponent
8	−0.6696077334198590
12	−0.6362863326795953
16	−0.6165741467010993
20	−0.603244670912252
24	−0.5934852417528157
28	−0.5859536198128706
32	−0.5799199948938484
36	−0.5749497141578801
40	−0.5707659045338731
Extrap. ∞	−0.499998(4)

continuously. This is an incommensurate phase belonging to the universality class of the gaussian model [12]. It is interesting to determine the singularity of the free energy as (h,v) approach Γ from the incommensurate regime. It is widely believed [2,3,10] that the free energy singularity should be governed by an exponent 3/2, but an exact calculation has been done by Lieb and Wu when $h=0$ only [7], in which case

$$f \sim c(\gamma,u)\left[v - v_c(\gamma,u,b=0)\right]^{3/2} .$$

Our calculation is an extension of Lieb's and Wu's method. We will apply it first to the ground state energy of the spin chain, and later extend if to the free energy of the statistical model.

Eqs. (2.9), (2.12) and (2.13) determine, through the solution of (2.11), e_0, y and h as functions of A and B. We suppose that such dependence is analytic and e_0, y and h can be expanded in powers of δA, δB as $A \to A+\delta A$, $B \to B+\delta B$. In making such hypothesis we rely on the fact that the points A, B around which one expands are far from the singularities of the inhomogeneous term $\xi(\alpha)$ in (2.11) and that the resulting expansion (see (4.3)-(4.5)) is consistent with the solution at $|b| \leqslant \gamma$ (see Section 2). A rigorous proof along the lines of [21] is beyond the scope of this paper.

Making explicit the dependence of $R(\alpha)$ on A, B by writing $R(\alpha;A,B)$ we have, from (2.12),

$$\partial_A y(A,B) = -\frac{2}{2\pi}\int_A^B d\alpha\, \partial_A R(\alpha;A,B) + \frac{2}{2\pi}R(A;A,B) ,$$

$$\partial_B y(A,B) = -\frac{2}{2\pi}\int_A^B d\alpha\, \partial_B R(\alpha;A,B) - \frac{2}{2\pi}R(B;A,B) ,$$

$$\delta y = \partial_A y(A,B)\delta A + \partial_B y(A,B)\delta B + O(\delta A^2, \delta B^2, \delta A\,\delta B) . \tag{4.1}$$

Likewise, the energy per site

$$e_0(A,B) = \cosh\gamma + \frac{1}{2\pi}\int_A^B d\alpha\, e(\alpha)R(\alpha;A,B) - Vy = \cosh\gamma - Vy + e_0^{(1)}(A,B)$$

yields the derivatives

$$\partial_A e_0^{(1)}(A,B) = \frac{1}{2\pi}\int_A^B d\alpha\, e(\alpha)\partial_A R(\alpha;A,B) - \frac{1}{2\pi}e(A)R(A;A,B)\,,$$

$$\partial_B e_0^{(1)}(A,B) = \frac{1}{2\pi}\int_A^B d\alpha\, e(\alpha)\partial_B R(\alpha;A,B) + \frac{1}{2\pi}e(B)R(B;A,B)\,,$$

$$\delta e_0(A,B) = \partial_A e_0^{(1)}(A,B)\delta A + \partial_B e_0^{(1)}(A,B)\delta B + O(\delta A^2, \delta B^2, \delta A\,\delta B)\,, \quad (4.2)$$

etc. Similar equations can be obtained for h, specializing (2.9) to the endpoints of the curve and taking the symmetric form

$$-4ih(A,B) = p^0(A) + p^0(B) - \frac{1}{2\pi}\int_A^B d\beta\, R(\beta;A,B)\Big[\Theta(A-\beta) + \Theta(B-\beta)\Big]$$

hence

$$-4i\partial_A h(A,B) = -\frac{1}{2\pi}\int_A^B d\beta\, \partial_A R(\beta;A,B)\Big[\Theta(A-\beta) + \Theta(B-\beta)\Big]$$
$$+R(A;A,B)\Big[1 + \frac{1}{2\pi}\Theta(B-A)\Big]\,,$$

$$-4i\partial_B h(A,B) = -\frac{1}{2\pi}\int_A^B d\beta\, \partial_B R(\beta;A,B)\Big[\Theta(A-\beta) + \Theta(B-\beta)\Big]$$
$$+R(B;A,B)\Big[1 + \frac{1}{2\pi}\Theta(B-A)\Big]\,,$$

etc. Equations for the derivatives of $R(\alpha;A,B)$ are readily obtained from (2.11)

$$\partial_A R(\alpha;A,B) + \frac{1}{2\pi}\int_A^B d\beta\, K(\alpha-\beta)\partial_A R(\beta;A,B) = \frac{1}{2\pi}K(\alpha-A)R(A;A,B)\,,$$

$$\partial_B R(\alpha;A,B) + \frac{1}{2\pi}\int_A^B d\beta\, K(\alpha-\beta)\partial_B R(\beta;A,B) = -\frac{1}{2\pi}K(\alpha-B)R(B;A,B)\,,$$

etc.

We have carried out these expansions to the third order in δA, δB. In principle they can be used for any A, B with $a = \pi, |b| \leqslant \gamma$, and the integrals computed by Fourier transform. However, as it is already evident from the first order terms, the expansions simplify considerably when carried out around $A_0 = -\pi \pm i\gamma, B_0 = \pi \pm i\gamma$, which are zeros of the dn function

$$R(A_0; A_0, B_0) = R(B_0; A_0, B_0) = 0\,.$$

The details of the expansion are lengthy but straightforward, so only the final form is of interest. Writing

$$\delta A = -\delta a + i\delta b\,, \qquad \delta B = \delta a + i\delta b$$

and considering first the expansion around $A_0 = -\pi - i\gamma, B_0 = \pi - i\gamma$, we have

$$\delta e_0 = 2c_2\left[(\delta a)^3 - 3\delta a(\delta b)^2\right] - V\delta y + \dots\,, \tag{4.3}$$

$$\delta y = -\frac{c_1}{\pi}\delta a\,\delta b + \frac{c_3}{\pi}\delta b(\delta a)^2 + \dots\,, \tag{4.4}$$

$$\delta h = \frac{c_1}{2}\left[(\delta a)^2 - (\delta b)^2\right] + \frac{c_3}{3}(\delta a)^3 + \dots \tag{4.5}$$

with

$$c_1 = k'\left(\frac{I(k)}{\pi}\right)^2 > 0\,,$$

$$\frac{c_2}{c_1} = \frac{\sinh\gamma}{3\pi}\left[\frac{1}{4} + \sum_{n>0}\frac{(-1)^n n\exp(-n\gamma)}{\cosh\gamma}\right] > 0\,,$$

$$\frac{c_3}{c_1} = \frac{1}{\pi}\sum_{n}\frac{\exp(-|n|\gamma)}{2\cosh\gamma n} > 0\,.$$

Notice that $\delta y = 0 = \delta e_0$ when $\delta a = 0$, as it should, since by taking $\delta a = 0$ and $\delta b > 0$ we reenter the 'flat phase'. It is also important to check that if $\delta a = 0$ there is no way to increase h by changing b, as already discussed in Section 2. An increase in h, when keeping y fixed at $y = 0$, can instead be achieved by $\delta a < 0, \delta b = 0$, which confirms the numerical findings presented in Section 2. A variation $\delta a > 0$ is ruled out a priori, because the periodicity of (2.3) in the real direction implies that rapidities are contained in the strip $-\pi \leqslant \mathrm{Re}(\alpha) \leqslant \pi$ and a cannot exceed π.

Another point to discuss is the reliability of (4.3)-(4.5) when $n > N/2$, that is $\delta y < 0$. The Bethe-ansatz equations for the symmetric six-vertex model are always discussed keeping $n \leqslant N/2$, since the $\mathbb{Z}_2$ symmetry of arrow reversal guarantees that the spectrum is the same when $N/2 < n \leqslant N$. It is not immediately clear what happens to (2.3) when $n > N/2$. As an example, consider the one-dimensional sector $S^z = -N$ ($n = N$), whose only eigenstate is $|\downarrow\downarrow\downarrow\dots\downarrow\rangle$. It is not obvious that (2.3) should have only one solution when the number of unknowns is N. To be on the safe side we will trust (4.3)-(4.5) only for $n \leqslant \frac{N}{2}$ ($y \geqslant 0$). In this case $\delta b \geqslant 0$ and $\delta a \leqslant 0$. To deal with the states at $n > \frac{N}{2}$ ($y < 0$), one must resort to (A.2), which implies

$$e_0(\gamma, h_c + \delta h, V, -y) = e_0(\gamma, -h_c - \delta h, -V, y)\,. \tag{4.6}$$

Hence it is necessary to consider also an expansion around $h = -h_c, y = 0$. This can be done evaluating (4.1) and the following equations at the endpoints $A_0' = -\pi + i\gamma, B_0' = \pi + i\gamma$. The result is that (4.3)–(4.5) still hold, with $\delta b > 0$ (< 0) if $\delta y > 0$ (< 0). A final observation about (4.3)–(4.5) is that it is legitimate to neglect higher order terms in (4.4) and (4.5). The parameters δa and δb are independent and there is no control over their relative magnitude, but the second order term in (4.5) is dominant unless $\delta a \simeq \pm\delta b$, in which case the third order term is certainly larger than all possible fourth order terms. Likewise, in (4.4), no term δa^n or δb^n is allowed since we know that $\delta y = 0$ if $\delta a = 0$ or $\delta b = 0$. Consequently, all higher order terms can certainly be neglected and one can further limit the expansion to

$$\delta y = -\frac{c_1}{\pi}\delta a\,\delta b\,.$$

Suppose now that h is kept fixed at h_c and $V \neq 0$. Then, from (4.5),

$$\delta b = \mp\delta a\,,$$

where the upper (lower) sign holds for $\delta y > 0$ (< 0). Consider first $\delta y > 0$. Then

$$\delta y = \frac{c_1}{\pi}\delta a^2\,,$$

$$\delta e_0(\delta a) = -4c_2\delta a^3 - \frac{Vc_1}{\pi}\delta a^2\,,$$

which has a minimum, when $V > 0$, at

$$\delta a_0 = -\frac{Vc_1}{6\pi c_2}$$

that yields

$$\delta e_0(h = h_c, V > 0) = -\frac{2}{c_2^2}\left(\frac{Vc_1}{6\pi}\right)^3.$$

Notice that no minimum occurs if $V < 0$. Instead, if we consider $\delta y < 0$, one has a minimum at

$$\delta a_0 = \frac{Vc_1}{6\pi c_2}$$

that yields

$$\delta e_0(h = h_c, V < 0) = \frac{2}{c_2^2}\left(\frac{Vc_1}{6\pi}\right)^3$$

when $V < 0$. Consequently,

$$e_0(h = h_c, V) = e_0(h = h_c, V = 0) - \frac{2}{c_2^2}\left(\frac{c_1}{6\pi}\right)^3 |V|^3\,,$$

$$\delta y = \mathrm{sgn}(V)\frac{c_1}{\pi}\left(\frac{Vc_1}{6\pi c_2}\right)^2$$

is the ground state energy singularity as one approaches the point $(h_c, V=0)$ along the V direction.

The case $V=0, \delta h \neq 0$ is more involved. We want $\delta h > 0$, in order to move into the incommensurate phase. From (4.3)–(4.5)

$$\delta b = \pm\sqrt{f(\delta a)}\,, \qquad f(\delta a) = \delta a^2 + \frac{2}{3}\frac{c_3}{c_1}\delta a^3 - \frac{2}{c_1}\delta h\,, \tag{4.7}$$

$$\delta y = -\frac{c_1}{\pi}\delta a(\pm\sqrt{f(\delta a)})\,, \tag{4.8}$$

$$\delta e_0(\delta a) = 2c_2\delta a\left(-2(\delta a)^2 - 2\frac{c_3}{c_1}(\delta a)^3 + \frac{6}{c_1}\delta h\right), \tag{4.9}$$

where the sign in (4.8) depends on whether we want $\delta y > 0$ or $\delta y < 0$. The variation δa must be negative and contained in a range where $f(\delta a)$ is non-negative, so if

$$f(\delta a_0) = 0\,, \qquad \delta a_0 = -\sqrt{\frac{2}{c_1}}(\delta h)^{1/2} + O(\delta h)\,,$$

we consider

$$\delta a \leqslant \delta a_0\,.$$

It is not difficult to see that there is a left neighborhood of δa_0 (of the order $\delta h^{1/2}$), where

(1) $f(\delta a)$ is positive.

(2) $\delta y(\delta a)$ is monotonic.

(3) $\delta e_0(\delta a)$ is decreasing.

Consequently, regardless of the sign in (4.8), $\delta a = \delta a_0$ is a local minimum of $\delta e_0(\delta a)$, which, incidentally, corresponds to $\delta y = 0$. Inserting δa_0 in (4.9),

$$e_0(h_c + \delta h, V=0) = e_0(h_c, V=0) - 2c_2\left(\frac{2}{c_1}\delta h\right)^{3/2}. \tag{4.10}$$

Although it is not obvious from the previous proof, $\delta y = 0$ is actually a stationary point for $\delta e_0(\delta y)$. In fact

$$\frac{\partial \delta e_0}{\partial \delta y} = (\partial\delta e_0/\partial\delta a)|_{\delta a_0} / (\partial\delta y/\partial\delta a)|_{\delta a_0}$$

and

$$\frac{\partial \delta y}{\partial \delta a} = \pm\left(-\frac{c_1}{\pi}\sqrt{f(\delta a)} - \frac{c_1}{2\pi}\delta a\frac{f'(\delta a)}{\sqrt{f(\delta a)}}\right)$$

becomes infinite at δa_0.

The calculation of the free energy singularity is a simple extension of this method. The variation of the ground state energy is now replaced by (see (2.23))

$$-\delta(F(u,\gamma,h,y) + vy) = -\delta F - \delta y(v_c + \delta v)\,.$$

The variation of F is computed by means of an expansion analogous to (4.1) and (4.2). To keep things simple we consider $d < \gamma - 2u$, which is certainly true for u sufficiently small, so that Λ_R dominates over Λ_L. The surprisingly simple result is that, like for the spin chain, the first non-zero contribution comes at the third order. The quantity to minimize is

$$2c_2'(\delta a^3 - 3\delta a\delta b^2) - \delta y\delta v\,,$$

where

$$c_2' = \frac{c_1}{6\pi}\left[\frac{1}{2} + \sum_{n>0}\frac{(-1)^n\cosh(\gamma(n-2u))}{\cosh(\gamma n)}\right] > 0\,,$$

which looks exactly like (4.3) provided $c_2 \to c_2'$ and $V \to \delta v$. The conclusions are therefore the same and the free energy leading singularities approaching (h_c, v_c) from the incommensurate phase are

$$f(u,\gamma,h_c+\delta h,v_c) = f(u,\gamma,h_c,v_c) - 2c_2'\left(\frac{2}{c_1}\delta h\right)^{3/2}\,,$$

$$f(u,\gamma,h_c,v_c+\delta v) = f(u,\gamma,h_c,v_c) - \frac{2}{c_2'^2}\left(\frac{c_1}{6\pi}\right)^3|\delta v|^3\,.$$

5. Discussion

It is interesting to speculate about the nature of the phase transition at (h_c, v_c) and compare it with what happens at the other points of Γ.

We have always worked in the assumption that a complete set of eigenstates exists for the transfer matrix. It is well known that correlation functions can be analysed through a spectral decomposition by inserting a complete set of transfer matrix eigenvectors in the correlator [29]. For the correlator of two vertical arrows along the same column one has, on a $N \times M$ lattice

$$\langle\alpha_{0,0}\ \alpha_{0,n}\rangle = \frac{\mathrm{Tr}\,(\sigma_0^z T^n \sigma_0^z T^{M-n})}{\mathrm{Tr}\,T^M} \overset{M\to\infty}{\longrightarrow} \sum_k \left|\langle 0|\sigma_0^z|k\rangle\right|^2 \left(\frac{\Lambda_k}{\Lambda_0}\right)^n \tag{5.1}$$

and for the correlation function of the same variables, but along the horizontal direction

$$\langle\alpha_{0,0}\ \alpha_{n,0}\rangle = \frac{\mathrm{Tr}\,(\sigma_0^z\sigma_n^z T^M)}{\mathrm{Tr}\,T^M} \overset{M\to\infty}{\longrightarrow} \langle 0|\sigma_0^z\sigma_n^z|0\rangle\,, \tag{5.2}$$

where we have denoted with $|0\rangle$ the eigenstate of the largest eigenvalue of the transfer matrix on a finite lattice of width N. Here $\sum_k$ denotes the sum over a complete set of eigenvectors of the transfer matrix. Eqs. (5.1) and (5.2) define, in the ordered phase within Γ, two correlation lengths that we will denote by ξ_v and ξ_h, respectively. We further consider a third correlator

$$\frac{\mathrm{Tr}\,(\sigma_0^x T^n \sigma_0^x T^{M-n})}{\mathrm{Tr}\, T^M} \xrightarrow{M\to\infty} \sum_k \left|\langle 0|\sigma_0^x|k\rangle\right|^2 \left(\frac{\Lambda_k}{\Lambda_0}\right)^n . \tag{5.3}$$

In terms of a statistical average, (5.3) introduces two spin flips on the 0th column at distance n (in the vertical direction) from each other. Eq. (5.3) defines a third length, say ξ_f, which, like ξ_v, applies to correlations in the vertical direction. It is useful to consider first what happens at $h = 0$. Since, obviously

$$\left[\sigma_n^z, \sum_{j=1}^N \sigma_j^z\right] = 0$$

and the ground state of the ordered phase lies in the sector $S^z = 0$, only this sector contributes to (5.1) and (5.2). Furthermore, v does not change the spectrum within a sector of fixed S^z, and it does not modify the eigenvectors which depend (as explicitly seen from the Bethe ansatz [7,8]) on γ and h only. We conclude that v has no effect whatsoever on the correlators (5.1) and (5.2), which remain those of the symmetric six-vertex model, until a level-crossing transition takes place at $v = v(\gamma, u, b = 0)$, as given by (2.25). Here the system moves into the gaussian incommensurate phase, and the ground state, even for small $\delta v = v - v\,(\gamma, u, b = 0)$ falls into a sector at $y \neq 0$ [7], hence with S^z of order N. The transition occurs without divergence of the lengths ξ_v and ξ_h which jump from the (finite) value of the symmetric six-vertex to infinity. On the contrary, the operator σ^x in (5.3) connects the ground state to the sectors $S_z = \pm 1$ that become gapless linearly in v at $v(\gamma, u, b = 0)$. The same happens to the spin chain at V given by Eq. (3.21). One expects that $\xi_f^{-1} \simeq v - v\,(\gamma, u, b = 0)$ [14]. Our conjecture is that this picture does not change when $-h_c < h < h_c$, and the level crossing transition persists with the same features along all Γ, up to the points (h_c, v_c) or $(-h_c, -v_c)$. This is confirmed by numerical analysis that reveals a scaling of the energy gap $\Delta E \simeq N^{-2}$ for all points on Γ except (h_c, v_c) and $(-h_c, -v_c)$. At (h_c, v_c) the correlation lengths ξ_v and ξ_h should diverge according to the following argument. The fact that in the sector $S^z = 0$, as found numerically in Section 3,

$$\lim_{h\to h_c^-} \Delta \ln \Lambda(S^z = 0, h, v_c) = 0$$

would suggest that $\xi_v(h)$ diverges as $h \to h_c^-$, but it is not sufficient to prove it. The fact that Λ_k in (5.1) are generally complex forces one to sum over a whole band of them because oscillations can affect the behavior of ξ_v [29] (the same caution should be applied when dealing with ξ_f). This in not doable until it is clarified what takes the place of strings in the sector under consideration. Nevertheless, one can look at $\xi_h(h)$, as $h \to h_c^-$. As shown in Section 4, it is possible to enter the gaussian phase at (h_c, v_c) while keeping the ground state at $y = 0$. From (2.10) $y = 0$ does not necessarily imply that $S^z = 0$ ($n = N/2$), since S^z can be non-zero but remain finite in the limit $N \to \infty$ and y would still be zero. Still it is tempting to conjecture that the ground state remains at $S^z = 0$, and this is confirmed by preliminary numerical results on the spin chain. Hence no level crossing occurs here, because the Perron–Frobenius theorem prevents it in a sector of fixed S^z, and the expectation value in (5.2) is taken with the same Bethe-ansatz eigenvector in the two phases. Since in the gaussian phase $\xi_h(h)$ is infinite, it must diverge as $h \to h_c^-$ (or $h \to -h_c^+$).

This argument applies to the ordered commensurate phase, but it does not explain the dispersion relation (3.17) nor the scaling (3.18). In the incommensurate phase, characteristic lengths can be defined in the horizontal and vertical direction which scale at the Prokovskii–Talapov transition, like [14]

$$l_v \simeq l_h^z . \tag{5.4}$$

In the usual setting, e.g. at the point $(h = 0, v = v\,(\gamma, u, b = 0))$, $z = 2$ and the spin-chain excitations in sectors with $S_z \neq 0$ become massless with the non-relativistic dispersion law $\Delta E \simeq \Delta P^2$. It appears that Eq. (3.17) might arise from a Prokovskii–Talapov transition when the two coordinate axes are interchanged and therefore $z = 1/2$. Yet the previous discussion indicates that the point (h_c, v_c) shows some peculiar features that do not appear at other points on Γ and that warrant further investigations.

After the first submission of the paper, Kim has proved analytically some of the numerical results presented here [30].

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Appendix A

We discuss here the symmetries of $\mathcal{H}$ and of the transfer matrix. Under the action of the (unitary) charge conjugation operator

$$C = \prod_{k=1}^{N} \sigma_k^x , \quad C = C^\dagger = C^{-1} ,$$

$\mathcal{H}$ transforms as

$$C\mathcal{H}(\gamma, h, V)C = \mathcal{H}(\gamma, -h, -V) . \tag{A.1}$$

Since

$$C \left(\sum_{j=1}^{N} \sigma_j^z \right) C = - \sum_{j=1}^{N} \sigma_j^z$$

the spectra of the sectors at fixed S^z are related by

$$\mathcal{S}(\gamma, h, V, S^z) = \mathcal{S}(\gamma, -h, -V, -S^z) . \tag{A.2}$$

The same symmetry operation can be applied to the transfer matrix, using the matrix form of C

$$\langle \underline{\alpha}, C\underline{\alpha}' \rangle = \prod_{k=1}^{N} \delta_{\alpha_k, -\alpha'_k} .$$

From (2.1) and the definition of the Botzmann weights it is elementary to see that

$$C\ T(\gamma, u, h, v)\ C|_{\underline{\alpha},\underline{\alpha}'} = T(\gamma, u, -h, -v)|_{\underline{\alpha},\underline{\alpha}'} , \tag{A.3}$$

which implies the relation between spectra

$$\mathcal{S}_{\mathrm{TM}}\{h, v, S^z\} = \mathcal{S}_{\mathrm{TM}}\{-h, -v, -S^z\} . \tag{A.4}$$

This symmetry manifests itself in the fact that the partition function

$$Z_{\mathrm{PF}}(h, v) = Z_{\mathrm{PF}}(-h, -v) .$$

As far as $\mathcal{H}$ is concerned, another symmetry is in effect, implemented by the space inversion operator (not to be confused with the momentum)

$$P|\alpha_1, \alpha_2, \ldots, \alpha_{N-1}, \alpha_N\rangle = |\alpha_N, \alpha_{N-1}, \ldots, \alpha_2, \alpha_1\rangle , \quad P^2 = 1 ,$$
$$P\ \mathcal{H}(\gamma, h, V) P = \mathcal{H}(\gamma, -h, V) .$$

Hence

$$CP\mathcal{H}(\gamma, h, V = 0) PC = \mathcal{H}(\gamma, h, V = 0) .$$

So at $V = 0$ the spin chain recovers the $\mathbb{Z}_2$ symmetry under spin reversal and the spectra at S^z and $-S^z$ are identical. It is noteworthy that the same is not true for the transfer matrix.

Appendix B

Our Hamiltonian, at $h = 0$, $V = 0$, can be written, neglecting a constant additive term

$$\mathcal{H} = -\frac{1}{2} \sum_{j=1}^{N} \left[\Delta \sigma_j^z \sigma_{j+1}^z + \sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y \right] \quad \text{with} \quad \Delta < -1 \tag{B.1}$$

and it is mapped onto the Hamiltonian (see, e.g. Ref. [24])

$$\mathcal{H}_G = \frac{1}{2} \sum_{j=1}^{N} \left[\Delta \sigma_j^z \sigma_{j+1}^z + \sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y \right] \quad \text{with} \quad \Delta > 1 \tag{B.2}$$

through a unitary transformation

$$\mathcal{H}_G = U\,\mathcal{H}\,U^{-1}\,, \qquad U = \prod_{j=1}^{N/2} \sigma^z_{2j-1}\,.$$

Consider the shift operator S of (2.6). Let $|\Psi_n, P\rangle$ be an eigenstate of $\mathcal{H}$ with momentum P and $S^z = \frac{N}{2} - n$

$$\frac{1}{2}\sum_{j=1}^{N} \sigma^z_j |\Psi_n, P\rangle = \left(\frac{N}{2} - n\right) |\Psi_n, P\rangle\,,$$

$$S|\Psi_n, P\rangle = \exp(-iP)|\Psi_n, P\rangle\,.$$

Define U_0 as

$$U_0|\Psi_n, P\rangle := \prod_{j=1}^{N} \sigma^z_j |\Psi_n, P\rangle = (-1)^n\ |\Psi_n, P\rangle\,.$$

Then, an eigenstate of $\mathcal{H}_G$ with the same energy is $U\ |\Psi_n, P\rangle$. Since

$$\begin{aligned} SU|\Psi_n, P\rangle &= \exp(-iP)SUS^{-1}|\Psi_n, P\rangle \\ &= \exp(-iP)\prod_{j=1}^{N/2}\sigma^z_{2j}|\Psi_n, P\rangle\,, \\ \exp(-iP)UU_0|\Psi_n, P\rangle &= \exp(-i(P + n\pi))U|\Psi_n, P\rangle \\ &= \exp(-i\overline{P})U|\Psi_n\rangle \end{aligned}$$

$U|\Psi_n, P\rangle$ has momentum $\overline{P} = P + n\pi$. Hence the ground state of (B.2) has momentum $\overline{P_0} = n_0\pi = \frac{N}{2}\pi$, while $P_0 = 0$. As to the excitations

$$\Delta\overline{P} = \Delta P + (n - n_0)\pi = \Delta P - \frac{N_h \pi}{2}\,.$$

Each hole carries an additional momentum $-\pi/2$, which implies

$$\Delta E = m_0\sqrt{1 - k^2\sin^2(\Delta P)} \quad \rightarrow \quad \Delta E = m_0\sqrt{1 - k^2\cos^2(\Delta P)}\,.$$

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