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Inhomogeneous Ising chain in a transverse field: finite-size scaling and asymptotic conformal spectrum

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Abstract. The quantum version of the Hilhorst-van Leeuwen model i.e. an inhomogeneous Ising model in a transverse field with a marginal perturbation of the bulk interaction varying like l^{-1} with the distance l from the surface is studied numerically on a finite chain with symmetric interactions using fermion techniques and finite-size scaling at the bulk critical point. The surface exponents for the energy and the magnetisation are respectively $x_e = 2\alpha+2$, $x_m = \alpha+\frac{1}{2}$ when $\alpha \geqslant \alpha_c$ and $x_e = -\alpha+\frac{1}{2}$, $x_m = 0$ and $x'_m = -\alpha-\frac{1}{2}$ when $\alpha \leqslant \alpha_c$ where $\alpha_c = -\frac{1}{2}$ is the critical value of the perturbation amplitude below which the surface becomes ordered at the bulk critical point. Although the magnetic exponents can be translated from the known classical values, the surface thermal exponents seem to be new. The excitation spectrum obtained in the continuum limit exhibits an asymptotic conformal behaviour. An analytic calculation of the leading finite-size corrections when $\alpha > \alpha_c$ and a test for the consistency of the numerical results when $\alpha \leqslant \alpha_c$ are given in the appendix.

1. Introduction

When an inhomogeneous perturbation is introduced in the semi-infinite two-dimensional Ising model with an interaction $K(l)$ varying with the distance l from the surface like:

$$K(l) = K(\infty) - \bar{A}/l^{y} \tag{1.1}$$

where $K(\infty)$ is the bulk interaction, depending on the value of the decay exponent $y>0$, one may get different surface critical behaviours. This is the Hilhorst-van Leeuwen model (Hilhorst and van Leeuwen 1981) which has been extensively studied in recent years (Burkhardt 1982a, Blöte and Hilhorst 1983, Burkhardt and Guim 1984, Burkhardt *et al* 1984, Blöte and Hilhorst 1985).

The y-dependence of the surface critical behaviour may be understood using a simple scaling argument (Burkhardt 1982b, Cordery 1982). Near the bulk critical point K^*, under a change of the length scale by a factor b, $K(l) - K^*$ transforms locally like:

$$\Re[K(l)-K^*] = K'(\infty) - \bar{A}'/l'^{y} - K^* = b^{y_t}[K(\infty) - \bar{A}/l^{y} - K^*] \tag{1.2}$$

where $l' = l/b$ and y_t is the bulk thermal exponent. Substracting the bulk renormalisation equation from equation (1.2), one gets the following transformation for the amplitude of the inhomogeneity:

$$\bar{A}' = b^{y_t - y}\bar{A}. \tag{1.3}$$

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For the two-dimensional Ising model, $y_t = 1$ and, when $y > 1$ the perturbation is irrelevant, an ordinary surface critical behaviour is obtained. When $y < 1$, the perturbation becomes relevant, the surface is ordered at the bulk critical point when $\bar{A} < 0$ and there is an anomalous decay of the surface correlations. When $y = 1$, the perturbation is marginal, the surface is ordered at the bulk critical point when $\bar{A}$ is lower than a critical value $\bar{A}_c$, the surface critical exponents vary with $\bar{A}$ with a change in their behaviour at $\bar{A}_c$.

On a square lattice with a constant interaction parallel to the surface K_1 and a varying perpendicular interaction $K_2(l)$ of the form given in equation (1.1), the exponents are simple functions of the parameter:

$$A = 4\bar{A}/\sinh[2K_2(\infty)]. \tag{1.4}$$

The critical value when $y = 1$ is

$$A_c = -1 \tag{1.5}$$

and the marginal magnetic surface exponent is

$$x_m = (A+1)/2 \qquad A \geqslant -1 \tag{1.6a}$$

$$x_m = 0, \qquad x'_m = -(A+1)/2 \qquad A \leqslant -1 \tag{1.6b}$$

where the value $x_m = 0$ below A_c is linked to the spontaneous surface magnetisation and $x'_m = \eta_\parallel/2$ gives the decay of the surface correlations towards their non-vanishing limit.

These results can be translated for the one-dimensional inhomogeneous Ising model in a transverse field using the extreme anisotropic limit ($K_2(\infty) \to 0$, $K_1 \to \infty$) of the two-dimensional problem (Kogut 1979). Then:

$$\bar{A} \simeq 1/2K_2(\infty)A \tag{1.7a}$$

$$K_2(l) \simeq K_2(\infty)(1 - A/2l^y) = \lambda(l)\tau \tag{1.7b}$$

where $\tau = e^{-2K_1}$ is the infinitesimal lattice spacing in the temporal direction and

$$\lambda(l) = \lambda(\infty)(1 - \alpha/l^y) \tag{1.8}$$

is the inhomogeneous coupling between first-neighbour spins along the semi-infinite quantum chain with:

$$\alpha = A/2 \tag{1.9}$$

and $K_2(\infty) = \lambda(\infty)\tau$. The critical value of the perturbation amplitude when $y = 1$ is $\alpha_c = -\frac{1}{2}$ and the magnetic surface exponents are:

$$x_m = \alpha + \tfrac{1}{2} \qquad \alpha_c \geqslant -\tfrac{1}{2} \tag{1.10a}$$

$$x_m = 0, \qquad x'_m = -\alpha - \tfrac{1}{2} \qquad \alpha_c \leqslant -\tfrac{1}{2}. \tag{1.10b}$$

The first value is in agreement with the result of a direct calculation of the surface magnetisation on the semi-infinite quantum Ising chain (Peschel 1984, Kaiser and Peschel 1989).

In the present work we present some results concerning the inhomogeneous Ising model in a transverse field on a finite chain with $y = 1$ i.e. in the marginal case. In section 2 the thermal and magnetic surface exponents are deduced from a numerical finite-size scaling study of chains of up to 180 spins. Although the leading surface magnetic exponent is known, the surface thermal exponents and correction to scaling exponents are new. In section 3 we calculate the excitation spectrum of the finite chain in the continuum limit. In section 4 we discuss these results and an exact finite-size scaling calculation is presented in the appendix.

2. Finite-size scaling study of the surface magnetisation and the surface energy

Let us consider a symmetric inhomogeneous Ising quantum chain with $L-1$ spins (L even) and Hamiltonian:

$$\mathfrak{H} = -\sum_{l=1}^{L-1} \sigma_z(l) - \lambda(\infty) \sum_{l=1}^{L-2} \Delta_i(l)\sigma_x(l)\sigma_x(l+1) \tag{2.1}$$

where the deviation from the bulk interaction is included in $\Delta_i(l)(i=1,2)$ such that:

$$\Delta_1(l) = 1-\alpha/l \qquad l<L/2 \tag{2.2a}$$

$$\Delta_2(l) = 1-\alpha/(L-l-1) \qquad l \geqslant L/2 \tag{2.2b}$$

and σ_x, σ_z are Pauli spin operators defined in the usual way:

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{2.3}$$

$\mathfrak{H}$ commutes with the parity operator

$$P = \prod_{l=1}^{L-1} \sigma_z(l) \tag{2.4}$$

allowing a classification of the eigenstates into the odd ($P=-1$) and even ($P=+1$) sectors. The Hamiltonian can be written as a quadratic form in fermion operators through a Jordan-Wigner transformation (Jordan and Wigner 1928):

$$c(l) = \prod_{j=1}^{l-1} [\exp \mathrm{i}\pi\sigma^+(j)\sigma^-(j)]\sigma^-(l) \tag{2.5}$$

and may be put in diagonal form

$$\mathfrak{H} = E_0 + \sum_k \Lambda_k \eta_k^+ \eta_k \tag{2.6}$$

where E_0 is the ground state energy, through a canonical transformation using the fermion operators (Lieb *et al* 1961):

$$\eta_k = \sum_l [g_{kl}c(l) + h_{kl}c^+(l)] \tag{2.7}$$

where the coefficients g and h are real. The excitation energies squared, Λ_k^2, satisfy the eigenvalue equation:

$$\bar{\bar{\Lambda}}\bar{\Phi}_k = \Lambda_k^2 \bar{\Phi}_k \tag{2.8}$$

and the excitation matrix $\bar{\bar{\Lambda}}$ is given by the product:

$$\bar{\bar{\Lambda}} = (\bar{\bar{A}} - \bar{\bar{B}})(\bar{\bar{A}} + \bar{\bar{B}}) \tag{2.9}$$

with:

$$\bar{\bar{A}} = -\begin{bmatrix} 2 & \lambda(1) & & & 0 \\ \lambda(1) & 2 & \lambda(2) & & \\ & \ddots & \ddots & \ddots & \\ & & \lambda(L-3) & 2 & \lambda(L-2) \\ 0 & & & \lambda(L-2) & 2 \end{bmatrix} \tag{2.10a}$$

and

$$\bar{\bar{B}} = \begin{bmatrix} 0 & -\lambda(1) & & & 0 \\ \lambda(1) & 0 & -\lambda(2) & & \\ & \ddots & \ddots & \ddots & \\ & & \lambda(L-3) & 0 & -\lambda(L-2) \\ 0 & & & \lambda(L-2) & 0 \end{bmatrix} \tag{2.10b}$$

At the bulk critical point $\lambda(\infty) = 1$, the normalised eigenvectors $\bar{\Phi}_k$ and the excitation energies Λ_k are solutions of the eigenvalue problem:

$$\Delta_i(l-1)\Phi_k(l-1) - [\Lambda_k^2/4 - 1 - \Delta_i^2(l-1)]\Phi_k(l) + \Delta_i(l)\Phi_k(l+1) = 0 \tag{2.11}$$

with the boundary conditions:

$$\Delta_1(0)\Phi_k(0) + \Delta_1^2(0)\Phi_k(1) = 0 \tag{2.12a}$$

$$\Delta_2(L-1)\Phi_k(L) = 0. \tag{2.12b}$$

The normalised eigenvectors $\bar{\Phi}_k$ and $\bar{\Psi}_k$ satisfy the following relations:

$$(\bar{\bar{A}} + \bar{\bar{B}})\bar{\Phi}_k = \Lambda_k \bar{\Psi}_k \tag{2.13a}$$

$$(\bar{\bar{A}} - \bar{\bar{B}})\bar{\Psi}_k = \Lambda_k \bar{\Phi}_k \tag{2.13b}$$

and may be related to the coefficients of the canonical transformation through:

$$\Phi_k(l) = g_{kl} + h_{kl} \tag{2.14a}$$

$$\Psi_k(l) = g_{kl} - h_{kl}. \tag{2.14b}$$

Using equation (2.5) one may write the energy operators:

$$\sigma_z(l) = 2c^+(l)c(l) - 1 \tag{2.15a}$$

$$\sigma_x(l)\sigma_x(l+1) = [c^+(l) - c(l)][c^+(l+1) + c(l+1)] \tag{2.15b}$$

and the magnetisation operator:

$$\sigma_x(l) = [c^+(l) + c(l)] \prod_{j=1}^{l-1} [1 - 2c^+(j)c(j)]. \tag{2.15c}$$

The following non-vanishing matrix elements may be used in the finite-size scaling study:

$$e_\varepsilon^z(l) = \langle\varepsilon|\sigma_z(l)|0\rangle \tag{2.16a}$$

$$e_\varepsilon^{xx}(l, l+1) = \langle\varepsilon|\sigma_x(l)\sigma_x(l+1)|0\rangle \tag{2.16b}$$

for the energy, and:

$$m_\sigma(l) = \langle\sigma|\sigma_x(l)|0\rangle \tag{2.16c}$$

for the magnetisation. In these expressions $|0\rangle$ is the ground-state which is even and

$$|\varepsilon\rangle = |kk'\rangle = \eta_k^+ \eta_{k'}^+ |0\rangle \qquad (k < k') \tag{2.17}$$

is a two-fermion even eigenstate. Using (2.7) and (2.14) one gets:

$$e_{kk'}^z(l) = \Phi_{k'}(l)\Psi_k(l) - \Phi_k(l)\Psi_{k'}(l) \tag{2.18a}$$

$$e_{kk'}^{xx}(l, l+1) = \Phi_{k'}(l+1)\Psi_k(l) - \Phi_k(l+1)\Psi_{k'}(l). \tag{2.18b}$$

On the first site we have to work with one-fermion excited states to get a non-vanishing matrix element for the magnetisation:

$$|\sigma\rangle = |k\rangle = \eta_k^+ |0\rangle \tag{2.19}$$

leading to:

$$m_k(1) = \Phi_k(1). \tag{2.20}$$

On the second site from the surface one may use either the one-fermion excited states (2.19) or the three-fermion excited states:

$$|\sigma\rangle = |kk'k''\rangle = \eta_k^+ \eta_{k'}^+ \eta_{k''}^+ |0\rangle \qquad k < k' < k'' \tag{2.21}$$

for which:

$$m_k(2) = \Phi_k(2) \sum_{k'} \Phi_{k'}(1)\Psi_{k'}(1) - \Phi_k(1) \sum_{k'} \Phi_{k'}(2)\Psi_{k'}(1) \tag{2.22a}$$

$$m_{kk'k''}(2) = \Phi_k(2) e_{k''k'}^z(1) + \Phi_{k'}(2) e_{kk''}^z(1) + \Phi_{k''}(2) e_{k'k}^z(1). \tag{2.22b}$$

If the excitations are numbered starting with $k = 0$ for the lowest one, the following finite-size behaviour is expected:

$$e_{01}^z(1) \sim e_{01}^{xx}(1, 2) \sim L^{-x_e} \tag{2.23a}$$

$$m_0(1) \sim L^{-x_m} \tag{2.23b}$$

$$m_1(1) \sim L^{-x'_m} \qquad \alpha \leqslant -\tfrac{1}{2}. \tag{2.23c}$$

The finite-size study has been performed on chains with sizes varying between $L = 20$ and 180 and the exponents deduced from log–log plots of the matrix elements against L and extrapolated to $L = \infty$. The results for the leading and correction to scaling exponents are shown on the figures 1-4. The accuracy is sufficient to allow us to conjecture analytic expressions for x_e and correction to scaling exponents.

When $\alpha \geqslant -\frac{1}{2}$ one gets:

$$x_m = \alpha + \tfrac{1}{2} \tag{2.24a}$$

$$x_e = 2\alpha + 2 \tag{2.24b}$$

and:

$$m_{012}(2) \sim L^{-(3\alpha + 9/2)} \tag{2.24c}$$

$$e_{12}^z(1) \sim e_{12}^{xx}(1, 2) \sim L^{-(2\alpha+2)} \tag{2.24d}$$

whereas with $\alpha \leqslant -\frac{1}{2}$:

$$x_m = 0 \qquad x'_m = -\alpha - \tfrac{1}{2} \tag{2.25a}$$

$$x_e = -\alpha + \tfrac{1}{2} \tag{2.25b}$$

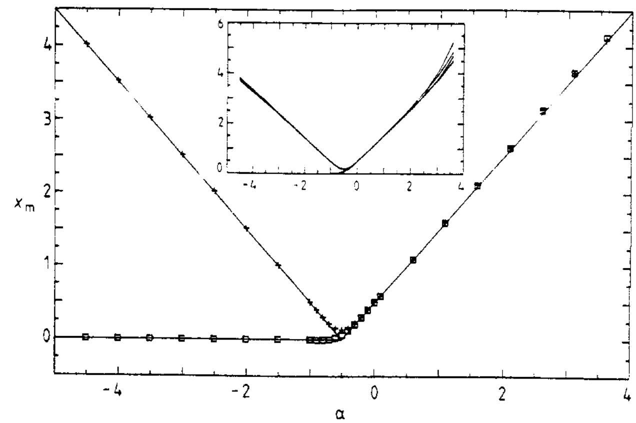

Figure 1. Variation of the surface magnetic exponents x_m (squares) and x'_m (crosses when $\alpha < -\frac{1}{2}$) with the perturbation amplitude α. The exponent $x_m(x'_m)$ is obtained through an extrapolation of the finite-size results for $m_0(1)$, $(m_1(1))$ on chains with length $L = 80$ to 180. The lines are the exact values (equations (2.24*a*) and (2.25*a*)) and the insert shows the convergence of the two-point fit results for five values of L between 80 to 180.

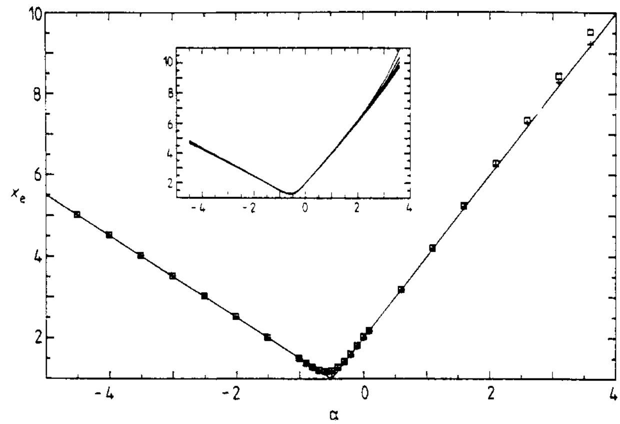

Figure 2. Variation of the surface energy exponent $x_e(\alpha)$ obtained through an extrapolation of the finite-size scaling results for $e_{01}^{-}(1)$ (squares) and $e_{01}^{xx}(1,2)$ (crosses) on chains with length $L = 80$ to 180. The lines give the conjectured analytical expressions (equations (2.24*b*) and (2.25*b*)) and the insert shows the convergence of the two-point fits.

and

$$m_{012}(2) \sim L^{-(2-2\alpha)} \tag{2.25c}$$

$$e_{12}^{-}(1) \sim e_{12}^{xx}(1,2) \sim L^{-(-2\alpha)}. \tag{2.25d}$$

3. Excitation spectrum in the continuum limit

In the finite-size scaling limit with $L \gg 1$, one may study the excitation spectrum in the continuum approximation introducing the variable $z = l/L$. With $\varphi(l) = (-1)^l \Phi(l)$ the

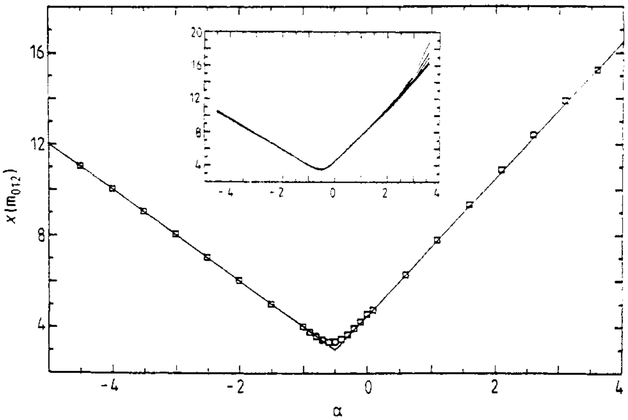

Figure 3. Variation of the surface magnetic correction to scaling exponent $x(m_{012})$ with α obtained through an extrapolation of the finite-size scaling results for $m_{012}(2)$ (equations (2.24c) and (2.25c)) on chains with length $L=80$ to 180. The lines correspond to the conjectured values.

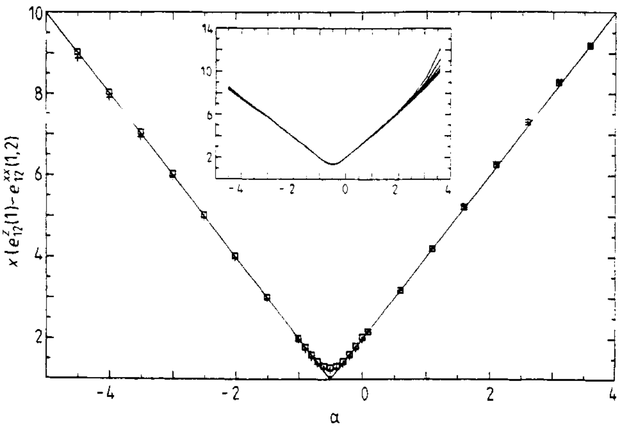

Figure 4. Variation of the surface energy correction to scaling exponent $x(e_{12}^{z})$ (squares) and $x(e_{12}^{xx})$ (crosses) with α obtained through an extrapolation of the finite-size scaling results for $e_{12}^{z}(1)$ and $e_{12}^{xx}(1,2)$ (equations (2.24d) and (2.25d)) on chains with length $L=80$ to 180. The lines correspond to the conjectured values.

finite-difference equation (2.11) may be rewritten as a second-order differential equation for the function $\varphi(z)$. Keeping terms up to $O(L^{-2})$ one gets:

$$\varphi_1''(z)+[(\Lambda L/2)^2-\alpha(\alpha-1)/z^2]\varphi_1(z)=0 \qquad 0<z<\tfrac{1}{2} \tag{3.1a}$$

$$(\alpha/z)\varphi_1(z)-\varphi_1'(z)|_{z=0}=0 \tag{3.1b}$$

for the first half of the chain and

$$\varphi_2''(z)+[(\Lambda L/2)^2-\alpha(\alpha+1)/(1-z)^2]\varphi_2(z)=0 \qquad \tfrac{1}{2}<z<1 \tag{3.2a}$$

$$\varphi_2(z)|_{z=1}=0 \tag{3.2b}$$

for the second half. The finite-difference equation (2.11) for $l=L/2$ leads to the continuity conditions:

$$\varphi_1(\tfrac{1}{2}) = \varphi_2(\tfrac{1}{2}) \tag{3.3a}$$

$$\varphi_1'(\tfrac{1}{2}) = \varphi_2'(\tfrac{1}{2}). \tag{3.3b}$$

Equations (3.1*a*) and (3.2*a*) are Bessel equations with particular solutions:

$$\varphi_1^{\pm}(z) \sim z^{1/2} J_{\pm(\alpha-1/2)}(cz) \tag{3.4a}$$

$$\varphi_2^{\pm}(z) \sim (1-z)^{1/2} J_{\pm(\alpha+1/2)}[c(1-z)] \tag{3.4b}$$

where $c = \Lambda L/2$. According to the z expansion of the Bessel function:

$$J_\nu(z) = z^\nu \sum_{k=0}^{\infty} \frac{(-1)^k z^{2k}}{k!\Gamma(\nu+k+1)2^{\nu+2k}} \tag{3.5}$$

the boundary condition (3.2*b*) for $z=1$ is satisfied by $\varphi_2^+(z)$ when $\alpha > -1$ and by $\varphi_2^-(z)$ when $\alpha < 0$. Assuming the continuity of the solution with α, one gets:

$$\varphi_2(z) = B(1-z)^{1/2} J_{\alpha+1/2}[c(1-z)] \qquad \alpha \geqslant -\tfrac{1}{2} \tag{3.6a}$$

$$\varphi_2(z) = B(1-z)^{1/2} J_{-(\alpha+1/2)}[c(1-z)] \qquad \alpha \leqslant -\tfrac{1}{2}. \tag{3.6b}$$

Using equation (3.4*a*) and the relations between Bessel functions and their derivatives (Abramowitz and Stegun 1970) the boundary condition for $z=0$ (equation (3.2*b*)) may be transformed into:

$$z^{1/2} J_{\pm(\alpha+1/2)}(cz) = 0. \tag{3.7}$$

So that, with the same assumption about the continuity with α as above, one gets

$$\varphi_1(z) = Az^{1/2} J_{\alpha-1/2}(cz) \qquad \alpha \geqslant -\tfrac{1}{2} \tag{3.8a}$$

$$\varphi_1(z) = Az^{1/2} J_{-(\alpha-1/2)}(cz) \qquad \alpha \leqslant -\tfrac{1}{2}. \tag{3.8b}$$

The continuity of $\varphi(z)$ and its derivatives for $z = \frac{1}{2}$ provides a linear system for A and B with non-vanishing solutions when the following relations are satisfied:

$$J^2_{\alpha-1/2}(c/2) = J^2_{\alpha+1/2}(c/2) \qquad \alpha \geqslant -\tfrac{1}{2} \tag{3.9a}$$

$$J^2_{-(\alpha-1/2)}(c/2) = J^2_{-(\alpha+1/2)}(c/2) \qquad \alpha \leqslant -\tfrac{1}{2} \tag{3.9b}$$

and the excitation energies Λ_k may be deduced from these relations.

Let us first look for low-lying excitations. When $\alpha \geqslant -\frac{1}{2}$ a small c expansion of equation (3.9*a*) obtained using (3.5) gives the lowest mode:

$$\Lambda_0 = 8(\alpha + \tfrac{1}{2})/L + \mathrm{O}(\alpha + \tfrac{1}{2})^2 \tag{3.10}$$

vanishing linearly with α at $\alpha_c = -\frac{1}{2}$. No such solution is obtained when $\alpha < -\frac{1}{2}$ so that one may expect that Λ_0 vanishes faster than L^{-1}.

Then up to $\mathrm{O}(L^{-2})$ equations (3.1*a*) and (3.2*a*) with $\Lambda = 0$ have power-law solutions and

$$\varphi_1(z) = Az^\alpha \tag{3.11a}$$

$$\varphi_2(z) = B(1-z)^{-\alpha} \tag{3.11b}$$

satisfy the boundary conditions when $\alpha < 0$, but continuity in α still requires $\alpha < -\frac{1}{2}$ for the occurence of a zero-mode. This solution is linked to the spontaneous surface magnetisation appearing below α_c. In order to normalise the eigenfunction one has to introduce a cut-off at $z = 1/L$ and then, with $\varphi(z)$ normalised to L^{-1}, one gets:

$$\varphi_1(1/L) \sim L^0 \tag{3.12}$$

i.e. an amplitude independent of the size of the system. This behaviour is related to the finite value of $\Phi_0(1)$ associated with the spontaneous surface magnetisation in the discrete formulation.

The asymptotic form of the spectrum at high excitation energies may be obtained using the z^{-1} expansion of the Bessel functions:

$$J_\nu(z) = (2/\pi z)^{1/2}[\cos(z - \pi\nu/2 - \pi/4) + \mathrm{O}(z^{-1})]. \tag{3.13}$$

Let us rewrite the eigenvalue equations (3.9) as:

$$J_p^2(c/2) = J_q^2(c/2) \tag{3.14}$$

with $p = \alpha - \frac{1}{2}$, $q = \alpha + \frac{1}{2}$ when $\alpha \geqslant -\frac{1}{2}$ and $p = -(\alpha - \frac{1}{2})$, $q = -(\alpha + \frac{1}{2})$ when $\alpha \leqslant -\frac{1}{2}$. With the expansion (3.13), one gets:

$$\sin[c - (p + q + 1)\pi/2] = 0 \tag{3.15}$$

so that

$$c = (p + q + 2k + 1)\pi/2 \tag{3.16}$$

and the asymptotic values of the excitation energies are

$$\Lambda_k = (2\pi/L)(\alpha + \tfrac{1}{2} + k) \qquad (\alpha \geqslant -\tfrac{1}{2}) \tag{3.17a}$$

$$\Lambda_0 = 0, \qquad \Lambda_{k+1} = (2\pi/L)(-\alpha + \tfrac{1}{2} + k) \qquad \alpha \leqslant -\tfrac{1}{2}. \tag{3.17b}$$

Comparing equation (3.17*a*) with equation (3.10), one may suspect that the spectrum begins with $k = 0$ when $\alpha \geqslant -\frac{1}{2}$, the factor 8 corresponding to 2π in the asymptotic spectrum and continuity with α requires also $k = 0, 1, 2\ldots$ in equation (3.17*b*). This is confirmed in figure 5 where the low-lying excitations on a chain with 180 spins are compared with the asymptotic values.

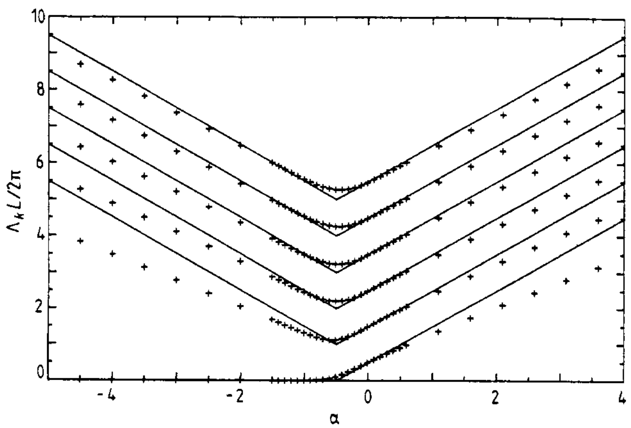

Figure 5. Variation of the first six excitations with α (crosses), as obtained on a chain with length $L = 180$, compared to the asymptotic spectrum (equations (3.17*a*) and (3.17*b*)). The first excitation vanishes when $\alpha < -\frac{1}{2}$.

4. Discussion

The study of the asymptotic spectrum in the preceding section was stimulated by a recent work of Igloi (Igloi 1989) in which the asymptotic spectrum of the asymmetric chain (with $\Delta_1(l)$ for all l in equation (2.1)) was studied. Since the symmetric chain we had used in the finite-size study appeared to be more appropriate to look at the surface critical behaviour we repeated the calculation in this case and we found that using the excitation energies given in equation (3.17), one may build the asymptotic conformal towers:

$$E_n - E_0 = (\pi/L)v_s x_n \tag{4.1}$$

where E_0 is the ground-state energy, $v_s = 2$ is the sound velocity, E_n are excited states constructed from the asymptotic excitations and x_n are critical dimensions associated with a scaling operator related to the dimension of a primary operator x_1 by $x_{n+1} = x_1 + n (n = 0, 1, 2, \dots)$. When $\alpha \geqslant -\frac{1}{2}$ the lowest dimension in the odd sector

$$x_{\rm m} = \alpha + \tfrac{1}{2} \tag{4.2}$$

gives the magnetisation exponent in agreement with (2.24*a*). One has to associate an odd number of excitations to build odd states so that the general expression for the scaling dimensions for odd operators is:

$$x^{\rm odd}(p,q) = (2p+1)\alpha + (2q+1)/2 \qquad p, q = 0, 1, 2, \dots . \tag{4.3}$$

The behaviour of $m_{012}(2)$ in equation (2.24*c*) corresponds to $x^{\rm odd}(1,4)$ which is the lowest dimension with three excitations since the allowed p and q values begin with $p = 1$, $q = 4$ in this case. In the even sector, always with $\alpha \geqslant -\frac{1}{2}$, the lowest dimension is:

$$x_{\rm e} = 2\alpha + 2 \tag{4.4}$$

in agreement with the finite-size conjecture of equation (2.24*b*). Since an even number of excitations is required to build even states, one gets the general expression:

$$x^{\rm even}(p,q) = 2p\alpha + q \qquad p = 1, 2, \dots, q = 2, 3, \dots . \tag{4.5}$$

When $\alpha \leqslant -\frac{1}{2}$ in the odd sector the lowest dimension is

$$x_{\rm m} = 0 \tag{4.6}$$

which may be associated with $\Lambda_0 = 0$. The next one $-\alpha + \frac{1}{2}$ differs from $x'_{\rm m} = -\alpha - \frac{1}{2}$ obtained through finite-size scaling. Taking Λ_0 into account, one gets the odd dimensions:

$$x^{\rm odd}(p,q) = -2p\alpha + q \qquad p = 1, 2, \dots, q = 2, 3, \dots \tag{4.7}$$

and the behaviour of $m_{012}(2)$ in equation (2.25*c*) corresponds to $x^{\rm odd}(1,2)$. Even dimensions are given by:

$$x^{\rm even}(p,q) = -(2p+1)\alpha + (2q+1)/2 \qquad p, q = 0, 1, 2, \dots \tag{4.8}$$

the lowest one giving $x_{\rm e} = -\alpha + \frac{1}{2}$. Using states built without taking Λ_0 into account leads to:

$$x^{\rm odd}(p,q) = -(2p+1)\alpha + (2q+1)/2 \qquad p, q = 0, 1, 2, \dots \tag{4.9}$$

$$x^{\rm even}(p,q) = -2p\alpha + q \qquad p = 1, 2, \dots, q = 2, 3, \dots \tag{4.10}$$

i.e. the same dimensions as above with a change in the parity. Curiously if the value $k=-1$ is retained in equation (3.17b), the allowed q values would begin with $q=-1$ in (4.9) and $q=0$ in (4.10) and $x'_{\mathrm{m}}=-\alpha-\frac{1}{2}$ would be obtained as $x^{\mathrm{odd}}(0,-1)$ whereas the behaviour of the energy operators in equation (2.25d) would correspond to $x^{\mathrm{even}}(1,0)$. Although the value $k=-1$ gives as required a non-negative value of the excitation energy when $\alpha\leqslant-\frac{1}{2}$, no state corresponding to this excitation appears in the spectrum (figure 5).

Our results are consistent with what may be called an asymptotic conformal behaviour of the model. It must be stressed that the Hamiltonian of equation (2.1) which was introduced for the finite-size scaling study is *not* the *conformal transformed* of the semi-infinite Hilhorst-van Leeuwen Hamiltonian. The conformally transformed system has been recently obtained (Burkhardt and Igloi 1990) by applying the $w(z)=L/\pi\ln z$ transformation (Cardy 1987) to the semi-infinite system. The transformed interaction is then:

$$\lambda(l)=\lambda(\infty)\left[1-\frac{\alpha}{(L/\pi)\sin[\pi l/L]}\right] \tag{4.11}$$

which gives back our model when $1/L$ and $1-l/L\ll 1$ i.e. far from the middle of the chain but avoids a cusp at $l=L/2$. The exact spectrum has been obtained in the continuum limit (Burkhardt and Igloi 1990) and coincide with our asymptotic spectrum, explaining the asymptotic conformal behaviour obtained in the present work.

For high positive α values, antiferromagnetic correlations appear near the surface and the excitation spectrum of the discrete model becomes quite complicated. A study of this domain is in progress.

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Appendix. Exact results for the finite-size scaling when $\alpha>-\frac{1}{2}$

In this appendix we calculate the size dependance of the surface properties of the discrete model at the bulk critical point $\lambda(\infty)=1$ when $\alpha>-\frac{1}{2}$ using a method previously introduced by Peschel in a study of the λ-dependance of the surface magnetisation of the semi-infinite inhomogeneous system (Peschel 1984).

In order to simplify the exposition we take an asymmetric interaction $\Delta_1(l)$ between the $L-1$ spins of the chain and study the properties of the surface at $l=1$. The symmetric model gives the same behaviour.

The leading contribution to $\Phi_k(l)$ may be obtained from the eigenvalue equation if one neglects the $O(L^{-2})$ contribution of Λ_k^2 in equation (2.11). With the boundary condition (2.12a), one gets a recursion relation for the components of Φ_k:

$$\Phi_k(l+1)\simeq-(1/\Delta_1(l))\Phi_k(l) \tag{A1}$$

leading to:

$$\Phi_k(l)=(-1)^{l-1}\Phi_k(1)\prod_{j=1}^{l-1}\Delta_1^{-1}(j). \tag{A2}$$

The eigenvector must be normalised so that:

$$\sum_{l=1}^{L-1} \Phi_k^2(l) = 1 = \Phi_k^2(1) \sum_{l=1}^{L-1} \sum_{j=1}^{l-1} \Delta_1^{-2}(j). \tag{A3}$$

The product may be expressed in terms of Γ-functions:

$$\prod_{j=1}^{l-1} \Delta_1^{-1}(j) = \prod_{j=1}^{l-1} (1-\alpha/j)^{-1} = [\Gamma(1-\alpha)\Gamma(l)]/\Gamma(l-\alpha) \tag{A4}$$

and for large l values, one may use the expansion:

$$\Gamma(z+b) = (2\pi)^{1/2}\, e^{-z} z^{z+b-1/2}[1+O(z^{-1})] \tag{A5}$$

to write:

$$\prod_{j=1}^{l-1} \Delta_1^{-2}(j) = \Gamma^2(1-\alpha) l^{2\alpha}[1+O(l^{-1})]. \tag{A6}$$

Changing the sum in (A3) into an integral and using the asymptotic expression of the product, with $\alpha > -\frac{1}{2}$ one gets:

$$\Phi_k(1) \simeq \Phi(1) = \frac{1}{\Gamma(l-\alpha)}\left(\int_0^L \mathrm{d}l\, l^{2\alpha}\right)^{-1/2} = \frac{\sqrt{2\alpha+l}}{\Gamma(l-\alpha)} L^{-(\alpha+1/2)} \tag{A7}$$

which is independent of the state k to this order and leads to $x_{\mathrm{m}} = \alpha + \frac{1}{2}$.

To get the surface energy, one needs $\Psi_k(1)$ given by:

$$\Psi_k(1) = -2/\Lambda_k[\Phi_k(1) + \Delta_1(1)\Phi_k(2)] \tag{A8}$$

according to equation (2.13a). From equations (2.11) and (2.12a) we have exactly:

$$\Phi_k(2) = (\Lambda_k^2/4 - 1)\Phi_k(1)/\Delta_1(1) \tag{A9}$$

where we keep the $O(L^{-2})$ contribution in the bracket since the leading term vanishes in equation (A8) and:

$$\Psi_k(1) = -(\Lambda_k/2)\Phi_k(1). \tag{A10}$$

Using equation (2.18a) one gets:

$$e^{z}_{kk'}(1) \sim \tfrac{1}{2}(\Lambda_{k'} - \Lambda_k)\Phi^2(1) \sim L^{-(2\alpha+2)}. \tag{A11}$$

The same behaviour is obtained for $e^{xx}_{kk'}(1,2)$ in equation (2.18b) so that $x_{\mathrm{e}} = 2\alpha + 2$ when $\alpha > -\frac{1}{2}$ in agreement with the numerical results.

With $m_{kk'k''}(2)$ given in equation (2.22b) although each of the three terms is of order $L^{-(3\alpha+5/2)}$ one may verify using (A11) that the sum of these leading contributions vanishes and the next term involves a factor $O(L^{-2})$ arising from the Λ_k^2 correction to $\Phi_k(2)$ so that $m_{kk'k''}(2) \sim L^{-(3\alpha+9/2)}$ in agreement with the results of figure 3.

Like in the case of the semi-infinite system (Peschel 1984) the method fails when $\alpha < -\frac{1}{2}$ where it gives the constant leading contribution to $\Phi_0(1)$ but does not predict the correct finite-size behaviour for $\Phi_{k\neq 0}(1)$. Nevertheless assuming $\Phi_{k\neq 0}(1) \sim L^{\alpha+1/2}$ in agreement with $x'_{\mathrm{m}} = -\alpha - \frac{1}{2}$ and using (A10) one gets:

$$\Psi_0(1) \sim O(L^{-1}),\ \Psi_{k\neq 0}(1) \sim L^{\alpha-1/2} \tag{A12}$$

and equation (2.18a) leads to $e^{z}_{01}(1) \sim L^{-(-\alpha+1/2)}$ so that the values of x_{e} and x'_{m} obtained for $\alpha \leqslant -\frac{1}{2}$ are mutually consistent. In the same way one gets $e^{z}_{12}(1) \sim L^{2\alpha}$ in agreement with equation (2.25d).

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