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Critical–off-critical interface in the Ising quantum chain and conformal invariance

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Abstract. The low-energy excitation spectrum of an Ising quantum chain in a transverse field which is critical ($h = J = 1$) for $1 \leq n \leq L/2$ and off-critical ($h \neq J$) for $L/2 < n \leq L$ is calculated up to $O(L^{-1})$. Interface critical exponents are determined numerically in the odd sector and exactly in the even sector using finite-size scaling. One gets an ordinary surface transition when $h > J$ and an extraordinary surface transition when $h < J$. The gap–exponent relation is verified, the mass gaps and the levels degeneracy are in agreement with conformal invariance.

1. Introduction

Using conformal invariance (Belavin *et al* 1984, Cardy 1987, Itzykson *et al* 1988) an infinite 2D system at its critical point may be mapped onto a strip with finite width L on which the lowest gaps of the Hamiltonian associated with the transfer operator in the extreme anisotropic limit (Kogut 1979, Henkel 1990) vanish as L^{-1} with amplitudes proportional to the scaling dimensions of the corresponding operators (Cardy 1984). Furthermore the energy spectrum displays tower-like structures with equidistant levels, the degeneracy of which is completely determined by conformal invariance.

Although translational and rotational invariance are in principle required, it has been shown that conformal invariance is preserved with localized defects (Henkel and Patkos 1987, 1988, Henkel *et al* 1989) and even for extended defects (Hinrichsen 1990) provided the defect configurations are commensurate. In the case of a long-range marginal inhomogeneity the gap–exponent relations are still verified (Burkhardt and Igloi 1990, Igloi *et al* 1990) and tower-like structures observed but the degeneracy of the levels is not yet understood.

In the present work, we show that conformal invariance still holds for a critical–off-critical interface in the 2D Ising model. This problem differs from the case considered previously (Hinrichsen 1990) where the extended defects were critical sectors in the plane with modified values of the critical interactions. We consider the quantum Ising chain Hamiltonian (figure 1)

$$H = -\frac{1}{2} \sum_{n=1}^{L/2} (\sigma^z(n) + \sigma^x(n)\sigma^x(n+1)) - \frac{1}{2} \sum_{n=L/2+1}^L (h\sigma^z(n) + J\sigma^x(n)\sigma^x(n+1)) \quad (1.1)$$

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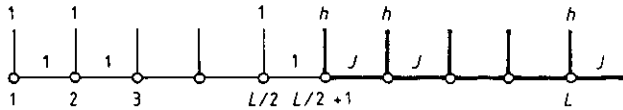


Figure 1. Critical-off-critical interface in the Ising quantum chain in a transverse field: h and $J(\neq 1)$ are the transverse field and the first-neighbour interaction in the off-critical part.

where σ^x and σ^z are Pauli spin operators, h and $J \neq 1$ the transverse field and the nearest-neighbour coupling in the off-critical part ($L/2 < n \leq L$). The prefactor in (1.1) has been introduced to ensure that the equations of motion are conformally invariant in the critical region (von Gehlen *et al* 1985). The chain length is assumed to be even and periodic boundary conditions are imposed with

$$\sigma^x(L+1) = \sigma^x(1). \tag{1.2}$$

This paper is organized as follows. In section 2 we calculate the low-energy excitation spectrum of H from which the energy levels in the two parity sectors are constructed. This is done using fermion techniques (Lieb *et al* 1961), the excitations being obtained as the solutions of an eigenvalue problem. In section 3 the corresponding eigenvectors are determined allowing us to get the dimension of the interface energy operator x_e through finite-size scaling. The dimension of the magnetization operator x_m is obtained through a numerical finite-size scaling study on the spin Hamiltonian. The results are discussed in section 4.

2. Low-energy excitation spectrum

The spin Hamiltonian (1.1) commutes with the parity operator $P = \prod_{n=1}^L \sigma^z(n)$ so that the eigenvalues are either even ($P = +1$) or odd ($P = -1$). Using the Jordan-Wigner transformation (Jordan and Wigner 1928) and omitting a constant term, one gets

$$H = - \sum_{n=1}^{L/2} [c^+(n)c(n) + \frac{1}{2}(c^+(n) - c(n))(c^+(n+1) + c(n+1))] - \sum_{n=L/2+1}^L \left[hc^+(n)c(n) + \frac{J}{2}(c^+(n) - c(n))(c^+(n+1) + c(n+1)) \right] \tag{2.1}$$

with the boundary conditions

$$c(n+1) = -Pc(1) \tag{2.2a}$$

$$c^+(n+1) = -Pc^+(1). \tag{2.2b}$$

This is a quadratic form in fermion operators in each parity sector which may be diagonalized through the Bogoliubov transformation (Lieb *et al* 1961):

$$\eta_p = \sum_{n=1}^L (g_{pn}c^+(n) + h_{pn}c(n)) \tag{2.3a}$$

$$\eta_p^+ = \sum_{n=1}^L (g_{pn}c(n) + h_{pn}c^+(n)) \tag{2.3b}$$

where the canonical operators satisfy the fermion anticommutation relations

$$\{\eta_p, \eta_{p'}\} = \{\eta_p^+, \eta_{p'}^+\} = 0 \tag{2.4a}$$

$$\{\eta_p, \eta_{p'}^+\} = \delta_{pp'}. \tag{2.4b}$$

In this way, one gets two diagonal Hamiltonians

$$H^{\pm} = \sum_p \Lambda_p^{\pm} (\eta_p^+ \eta_p - \frac{1}{2}) \quad (2.5)$$

one for each parity sector and the even (odd) eigenstates of H correspond to the even (odd) eigenstates of $H^{+(-)}$ whereas the remaining states acquire physical meaning only for antiperiodic boundary conditions.

Introducing the normalized eigenvectors

$$\phi_p(n) = (-1)^n (g_{pn} + h_{pn}) \quad (2.6a)$$

$$\psi_p(n) = (-1)^n (g_{pn} - h_{pn}) \quad (2.6b)$$

related through

$$-h(n)\phi_p(n) + J(n)\phi_p(n+1) = \Lambda_p^{\pm} \psi_p(n) \quad (2.7)$$

with

$$h(n) = J(n) = 1 \quad \left(n = 1, \frac{L}{2} \right) \quad (2.8a)$$

$$h(n) = h \quad \left(n = \frac{L}{2} + 1, L \right) \quad (2.8b)$$

$$J(n) = J \quad \left(n = \frac{L}{2} + 1, L - 1 \right) \quad (2.8c)$$

$$J(L) = -PJ \quad (2.8d)$$

the $(\Lambda_p^{\pm})^2$ are solutions of the eigenvalue problem

$$h(n-1)J(n-1)\phi_p(n-1) + ((\Lambda_p^{\pm})^2 - h^2(n) - J^2(n-1))\phi_p(n) + h(n)J(n)\phi_p(n+1) = 0 \quad (2.9)$$

with $J(0) = J(L)$ and the same notations as above. In the critical part ($n = 2$ to $L/2$) one gets

$$\phi_{1p}(n-1) + [(\Lambda_p^{\pm})^2 - 2]\phi_{1p}(n) + \phi_{1p}(n+1) = 0 \quad (2.10)$$

so that

$$\phi_{1p}(n) = A e^{ikn} + B e^{-ikn} \quad (2.11)$$

and

$$(\Lambda_p^{\pm})^2 = 4 \sin^2 \frac{k}{2} \quad (2.12)$$

whereas in the off-critical part ($n = L/2 + 2$ to $L - 1$):

$$hJ\phi_{2p}(n-1) + [(\Lambda_p^{\pm})^2 - h^2 - J^2]\phi_{2p}(n) + hJ\phi_{2p}(n+1) = 0 \quad (2.13)$$

and the components of the eigenvectors are given by

$$\phi_{2p}(n) = C e^{qn} + D e^{-qn} \quad (2.14)$$

with:

$$\cosh q = \frac{h^2 + J^2 - (\Lambda_p^{\pm})^2}{2hJ} \quad (2.15)$$

The quantization of the eigenvalues (2.12) is imposed by the boundary conditions

$$\phi_{1p}(0) + (J^2 - 1)\phi_{1p}(1) = -PhJ\phi_{2p}(L) \quad (2.16a)$$

$$\phi_{1p}\left(\frac{L}{2} + 1\right) = \phi_{2p}\left(\frac{L}{2} + 1\right) \quad (2.16b)$$

$$\phi_{1p}(1) = -P\phi_{2p}(L + 1) \quad (2.16c)$$

$$(h^2 - 1)\phi_{1p}\left(\frac{L}{2} + 1\right) + \phi_{1p}\left(\frac{L}{2} + 2\right) = hJ\phi_{2p}\left(\frac{L}{2} + 2\right) \quad (2.16d)$$

leading to the linear system

$$[1 + (J^2 - 1)e^{ik}]A + [1 + (J^2 - 1)e^{-ik}]B + PhJ e^{qL}C + PhJ e^{-qL}D = 0 \quad (2.17a)$$

$$e^{ik(L/2+1)}A + e^{-ik(L/2+1)}B - e^{q(L/2+1)}C - e^{-q(L/2+1)}D = 0 \quad (2.17b)$$

$$e^{ik}A + e^{-ik}B + P e^{q(L+1)}C + P e^{-q(L+1)}D = 0 \quad (2.17c)$$

$$[(h^2 - 1)e^{ik(L/2+1)} + e^{ik(L/2+2)}]A + [(h^2 - 1)e^{-ik(L/2+1)} + e^{-ik(L/2+2)}]B - hJ e^{q(L/2+2)}C - hJ e^{-q(L/2+2)}D = 0. \quad (2.17d)$$

The secular equation reads:

$$\begin{aligned} 2PhJ \sin k \sinh q + (J^2 - 1)(h^2 - 1) \sin \frac{kL}{2} \sinh \frac{qL}{2} + hJ(2 - h^2 - J^2) \sin \frac{kL}{2} \sinh \left(\frac{qL}{2} - q\right) \\ + h^2 J^2 \sin \frac{kL}{2} \sinh \left(\frac{qL}{2} - 2q\right) + (h^2 + J^2 - 2) \sin \left(\frac{kL}{2} + k\right) \sinh \frac{qL}{2} \\ - 2hJ \sin \left(\frac{kL}{2} + k\right) \sinh \left(\frac{qL}{2} - q\right) + \sin \left(\frac{kL}{2} + 2k\right) \sinh \frac{qL}{2} = 0. \end{aligned} \quad (2.18)$$

Looking for the critical modes $\Lambda_p^\pm \sim O(L^{-1})$, equation (2.15) gives

$$\cosh q = \frac{h^2 + J^2}{2hJ} + O(L^{-2}) \quad (2.19a)$$

$$\sinh q = \frac{|h^2 - J^2|}{2hJ} + O(L^{-2}) \quad (2.19b)$$

and equation (2.18) reduces to

$$k \cos \frac{kL}{2} \sinh \frac{qL}{2} [|h^2 - J^2| + O(L^{-2})] = 0 \quad (2.20)$$

so that, using (2.12), non-vanishing solutions are obtained when

$$|\Lambda_p^\pm| = \frac{2\pi}{L} \left(p + \frac{1}{2}\right) + O(L^{-2}) \quad (p = 0, 1, 2, \dots). \quad (2.21)$$

To this order in L^{-1} the same excitations are obtained in the two parity sectors. From equation (2.5) the ground-state energy of H^\pm is

$$E_0^\pm = -\frac{1}{2} \sum_p |\Lambda_p^\pm| \quad (2.22)$$

and higher levels are obtained by adding fermions to the ground state with a change of the parity for an odd number of excitations. Through a comparison with tridiagonalization results for the spin Hamiltonian (figure 2), one finds that the ground state of

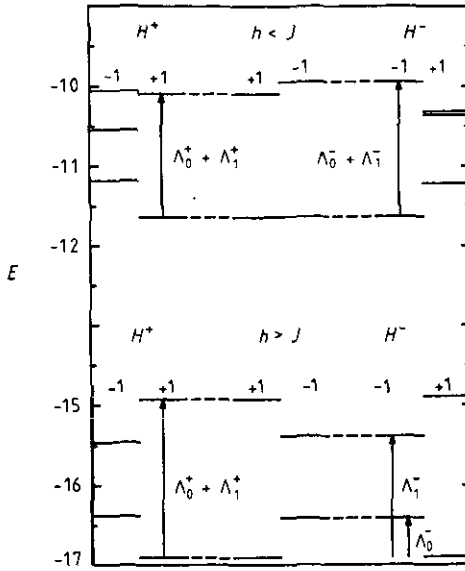


Figure 2. Construction of the spectrum of H from the even levels of H^+ and the odd levels of H^- . The central spectrum has been obtained through tridiagonalization of the spin Hamiltonian ($L = 10, J = 1$, top $h = 0.5$, bottom $h = 2.0$). The ground state of H^- is odd when $h < J$.

H^+ is always even whereas for H^- it is even when $h/J > 1$ and odd when $h/J < 1$. This last result is linked with the presence of a negative excitation $\Lambda_0^- < 0$ when $h/J < 1$. Then the ground state contains one fermion and $|\Lambda_0^-|$ may be reinterpreted as a hole excitation energy. The same thing happens for the homogeneous system in the ordered phase (Pfeuty 1970). Since equation (2.21) only gives the critical modes, we have to study numerically the behaviour of the gap between the two ground states. It turns out that $E_0^- - E_0^+$ vanishes exponentially with L as shown in figure 3.

The ground state of H is always even and $E_0 = E_0^+$. Higher levels in the even sector are constructed by adding an even number of excitations and one gets the mass gaps

$$E_r^+ - E_0 = \frac{2\pi}{L} r + O(L^{-2}) \quad r = 2, 3, 4, \dots \tag{2.23}$$

when $h \neq J$.

Since the ground state of H^- is even when $h > J$, an odd number of excitations is needed to get the energy levels of H in the odd sector and

$$E_r^- - E_0 = \frac{2\pi}{L} (\frac{1}{2} + r) + O(L^{-2}) \quad r = 0, 1, 2, \dots h > J. \tag{2.24}$$

When $h < J$, the ground state of H^- is odd and belongs to the spectrum of H . Up to $O(L^{-1})$ this state is degenerate with the ground state, a behaviour which is related to the onset of long-range order for the off-critical part in the thermodynamic limit. Higher odd states of H are obtained with an even number of excitations so that

$$E_r^- - E_0 = \frac{2\pi}{L} r + O(L^{-2}) \quad r = 0, 2, 3, \dots \quad h < J. \tag{2.25}$$

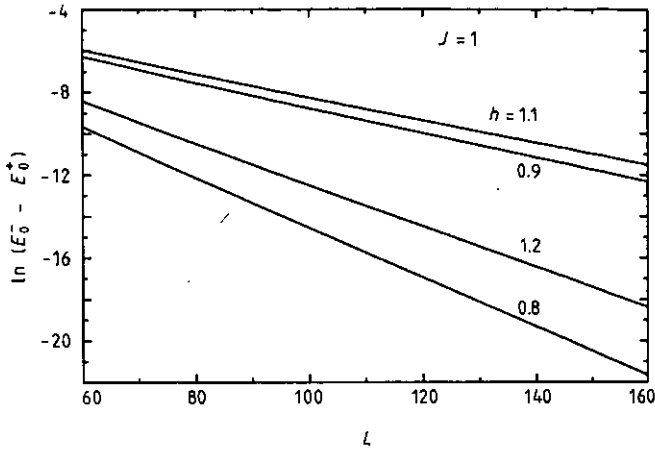


Figure 3. Variation of logarithm of the gap between the ground states of H^+ and H^- as a function of the chain length L for different values of the transverse field in the off-critical part and $J = 1$.

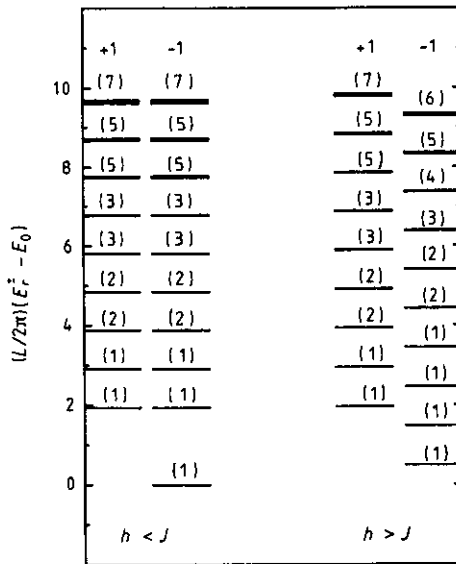


Figure 4. Mass gaps and degeneracy of the levels in the two parity sectors of H for a chain with length $L = 140$, $J = 1$, $h = 0.5$, (left) and 2.0 (right).

The mass gaps and the levels degeneracy of H for a chain with length $L = 140$ are shown in figure 4.

3. Eigenvectors and finite-size scaling

The magnetization operator $\sigma^x(1)$ anticommutes with the parity operator whereas the energy operator $\sigma^z(1)$ commutes. It follows that one may deduce their scaling

dimensions x_m and x_e from the finite-size behaviour of the following matrix elements (Barber 1983, Henkel 1990):

$$m(1) = \langle \sigma | \sigma^x(1) | 0 \rangle \sim L^{-x_m} \tag{3.1a}$$

$$e(1) = \langle \varepsilon | \sigma^z(1) | 0 \rangle \sim L^{-x_e} \tag{3.1b}$$

where $|0\rangle$ is the ground state, $|\sigma\rangle$ the first odd excited state and $|\varepsilon\rangle$ the first even excited state of H . Since $|0\rangle$ and $|\sigma\rangle$ belong to different parity sectors, the Lanczos tridiagonalization method has been used to determine x_m on chains with lengths $L = 4-14$. The results shown in figure 5(a) are consistent with

$$x_m = \frac{1}{2} \quad h > J \tag{3.2a}$$

$$x_m = 0 \quad x'_m = 2 \quad h < J \tag{3.2b}$$

where x'_m , governing the decay of the spin-spin correlations along the interface when the off-critical half-space is ordered, is obtained with the next odd excited state of H in equation (3.1a) (figure 5(b)).

Fermion techniques may be used to study $e(1)$, since then both states belong to the even sector. With

$$|\varepsilon\rangle = \eta_0^+ \eta_1^+ |0\rangle \tag{3.3a}$$

$$\sigma_z(1) = 2c^+(1)c(1) - 1 \tag{3.3b}$$

equations (2.3) and (2.6) lead to

$$e(1) = \phi_1(1)\psi_0(1) - \phi_0(1)\psi_1(1). \tag{3.4}$$

Let

$$X = \alpha \Delta_X \quad (X = A, B, C, D) \tag{3.5}$$

then the first three equations of the linear system (2.17) may be rewritten as

$$[1 + (J^2 - 1) e^{-ik}] \frac{\Delta_B}{\Delta_A} + PhJ e^{qL} \frac{\Delta_C}{\Delta_A} + PhJ e^{-qL} \frac{\Delta_D}{\Delta_A} = -[1 + (J^2 - 1) e^{ik}] \tag{3.6a}$$

$$-e^{-ik(L/2+1)} \frac{\Delta_B}{\Delta_A} + e^{q(L/2+1)} \frac{\Delta_C}{\Delta_A} + e^{-q(L/2+1)} \frac{\Delta_D}{\Delta_A} = e^{ik(L/2+1)} \tag{3.6b}$$

$$e^{-ik} \frac{\Delta_B}{\Delta_A} + P e^{q(L+1)} \frac{\Delta_C}{\Delta_A} + P e^{-q(L+1)} \frac{\Delta_D}{\Delta_A} = -e^{ik} \tag{3.6c}$$

where, for critical excitations, the Δ_X are the following determinants:

$$\Delta_A = P e^{qL/2} [1 + \frac{1}{2}(J^2 - h^2 - 2 + |h^2 - J^2|) e^{-ik}] [1 + O(L^{-2})] \tag{3.7a}$$

$$\Delta_B = -\Delta_A^* \tag{3.7b}$$

$$\Delta_C = -2ik e^{-q(L/2+1)} [1 + O(L^{-2})] \tag{3.7c}$$

$$\Delta_D = 2iP(-1)^p e^{qL} (e^q J^2 - hJ) [1 + O(L^{-2})]. \tag{3.7d}$$

Using equations (2.11), (2.19), (3.5) and (3.7), after some algebra, one gets

$$\phi_{1p}(n) = i\alpha P e^{qL/2} [2 \sin kn + (J^2 - h^2 - 2 + |h^2 - J^2|) \sin k(n-1)] [1 + O(L^{-2})] \tag{3.8a}$$

$$\phi_{2p}(n) = 2i\alpha [(-1)^p P (e^q J^2 - hJ) e^{q(L-n)} - k e^{q(n-L/2-1)}] [1 + O(L^{-2})] \tag{3.8b}$$

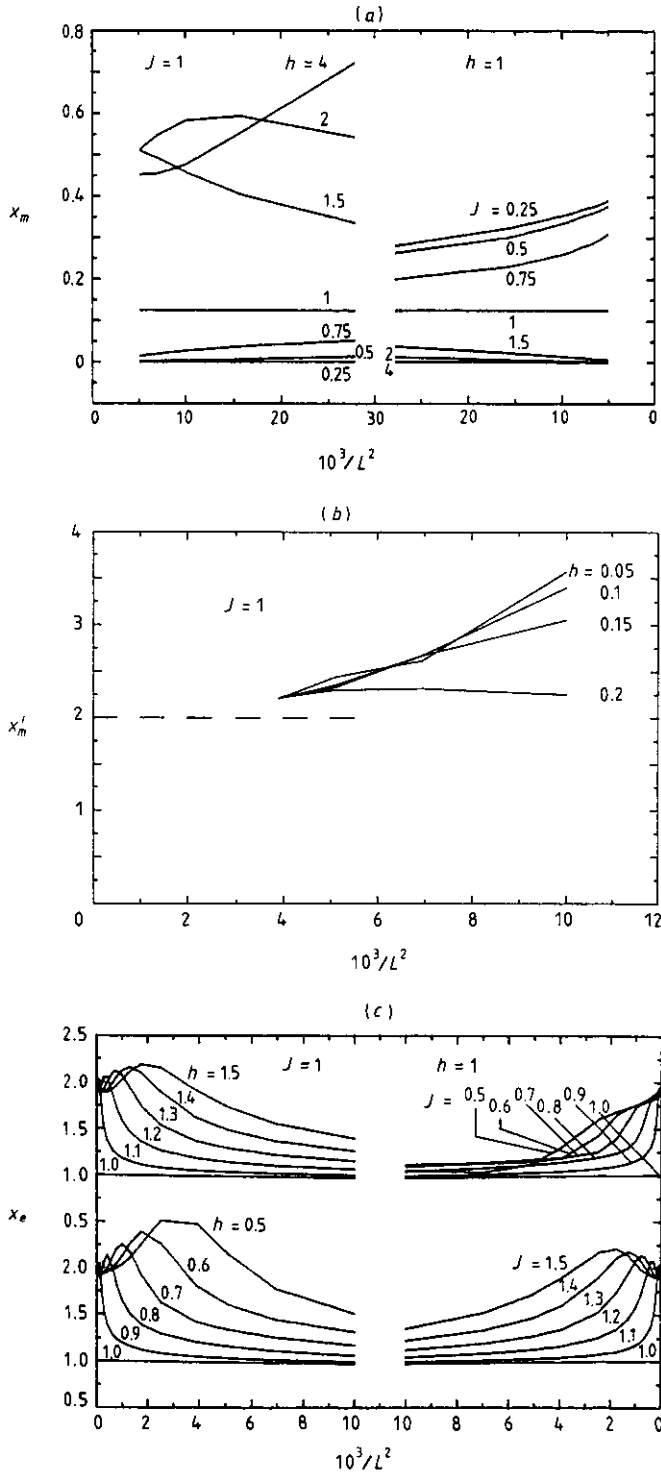


Figure 5. Critical exponents obtained through finite-size scaling: (a) x_m ($L=4, 14$), (b) x'_m ($L=8, 16$), (c) x_c ($L=10, 180$).

and

$$\sum_{n=1}^{L/2} |\phi_{1p}(n)|^2 = \begin{cases} \alpha^2 e^{qL} k^2 L [1 + O(L^{-1})] & h > J \\ \alpha^2 e^{qL} (J^2 - h^2)^2 L [1 + O(L^{-1})] & h < J \end{cases} \quad (3.9)$$

whereas

$$\sum_{n=L/2+1}^L |\phi_{2p}(n)|^2 = \begin{cases} 8\alpha^2 e^{qL} J^2 (h^2 - J^2)^{-1} & h > J \\ 8\alpha^2 e^{qL} J^2 (J^2 - h^2) & h < J \end{cases} \quad (3.10)$$

so that, for critical excitations, the contribution of the off-critical part to the norm of the eigenvectors may be ignored and one gets

$$\alpha = \begin{cases} e^{-qL/2} k^{-1} L^{-1/2} [1 + O(L^{-1})] & h > J \\ e^{-qL/2} (J^2 - h^2)^{-1} L^{-1/2} [1 + O(L^{-1})] & h < J. \end{cases} \quad (3.11)$$

Equations (2.7) and (3.8a) lead to

$$\phi_p(1) = \begin{cases} 2iPL^{-1/2} + O(L^{-3/2}) & h > J \\ 2i\pi P(2p+1)(J^2 - h^2)^{-1} L^{-3/2} + O(L^{-5/2}) & h < J \end{cases} \quad (3.12a)$$

$$\psi_p(1) = \begin{cases} -2i\pi P(2p+1)L^{-3/2} + O(L^{-5/2}) & h > J \\ 2iPL^{-1/2} + O(L^{-3/2}) & h < J \end{cases} \quad (3.12b)$$

and finally

$$e(1) = \begin{cases} -8\pi L^{-2} + O(L^{-3}) & h > J \\ -8\pi (J^2 - h^2)^{-1} L^{-2} + O(L^{-3}) & h < J \end{cases} \quad (3.13)$$

so that

$$x_e = 2 \quad h \neq J. \quad (3.14)$$

These values have been confirmed by a numerical study on chains with lengths $L = 10-180$ (figure 5(c)).

4. Discussion

The scaling dimensions x_e , x_m and x'_m associated with the critical-off-critical interface, obtained through finite-size scaling coincide with the surface exponents of the 2D Ising model either with free boundary conditions (ordinary transition) when $h > J$ (Binder 1983) or fixed boundary conditions (extraordinary transition) when $h < J$ (Burkhardt 1985).

The conformal algebra associated with the critical 2D Ising model is the Virasoro algebra with central charge $c = \frac{1}{2}$ (Belavin *et al* 1984, Cardy 1987). The lowest weights Δ_Φ of the irreducible representations giving the conformal dimensions of the primary fields Φ are $\Delta_\Phi = 0, \frac{1}{2}, \frac{1}{16}$. For free or fixed boundary conditions, the conformal towers

are constructed from the lowest weights and their descendants (von Gehlen and Rittenberg 1986, Cardy 1986):

$$E_r^\phi - E_0 = \frac{\pi}{l} (\Delta_\phi + r) \quad (4.1)$$

and the levels degeneracy $d(\Delta_\phi, r)$, given in table 1, can be computed from the character functions of the Virasoro algebra (Rocha-Caridi 1985).

Table 1. Lowest weights Δ_ϕ of the irreducible representations of the Virasoro algebra with central charge $c = \frac{1}{2}$ and degeneracy $d(\Delta_\phi, r)$ of the levels $\Delta_\phi + r$ in the conformal towers.

Δ_ϕ	r										
	0	1	2	3	4	5	6	7	8	9	10
0	1	0	1	1	2	2	3	3	5	5	7
$\frac{1}{2}$	1	1	1	1	2	2	3	4	5	6	8
$\frac{1}{16}$	1	1	1	2	2	3	4	5	6	8	10

With the critical-off-critical system, l is the width $L/2$ of the critical part so that the prefactors in equations (2.23), (2.24) and (2.25) are in agreement with equation (4.1). The energy spectrum in the even sector of H , when $h \neq J$, corresponds to the conformal tower with $\Delta_\phi = 0$ starting with the second descendant and one recovers $x_e = 2$ which is common to the ordinary and the extraordinary transitions (figure 6(c)). In the odd sector when $h > J$, we get the conformal tower of the magnetization operator with $\Delta_\phi = x_m = \frac{1}{2}$, whereas when $h > J$, $\Delta_\phi = x_m = 0$ so that the tower begins with $r = 0$ in equation (4.1). The first descendant does not appear since $d(0, 1) = 0$ in table 1 and the second gives $x'_m = 2$ (figures 6(a) and 6(b)). Although when $h < J$ the exponents of the extraordinary transition are those obtained with fixed boundary conditions (Cardy 1986), here the Z_2 symmetry is not broken by the boundary conditions and we get two degenerate odd and even sectors.

We have worked with constant values of h and J on the off-critical part of the chain. It must be emphasized that these constant values cannot be obtained through the conformal mapping $w = L/2\pi \ln z$ of the infinite plane onto the strip. Let $\Delta t(z)$, with scaling dimension $y_e = 1$, be the deviation from criticality on the off-critical half-space on the infinite plane. With $z = \rho e^{i\theta}$, the local dilatation is

$$b(z) = |w'(z)|^{-1} = \frac{2\pi\rho}{L} \quad (4.2)$$

so that

$$\Delta t(w) = b(z)^{y_e} \Delta t(z) = \frac{2\pi\rho}{L} \Delta t(z) \quad (4.3)$$

and we have to take $\Delta t(z) \sim L/\rho$ in order to get a constant deviation from criticality on the strip. The L -dependence of the interaction on the plane is clearly not acceptable.

One might use the conformal mapping after a renormalization of the plane giving a flow towards either the high- or the low-temperature fixed point in the off-critical part together with an irrelevant interfacial perturbation and leading to either $J/h = 0$ or $h/J = 0$ on the strip. A renormalization of the strip with either $h > J$ or $h < J$ leads to the same behaviour.

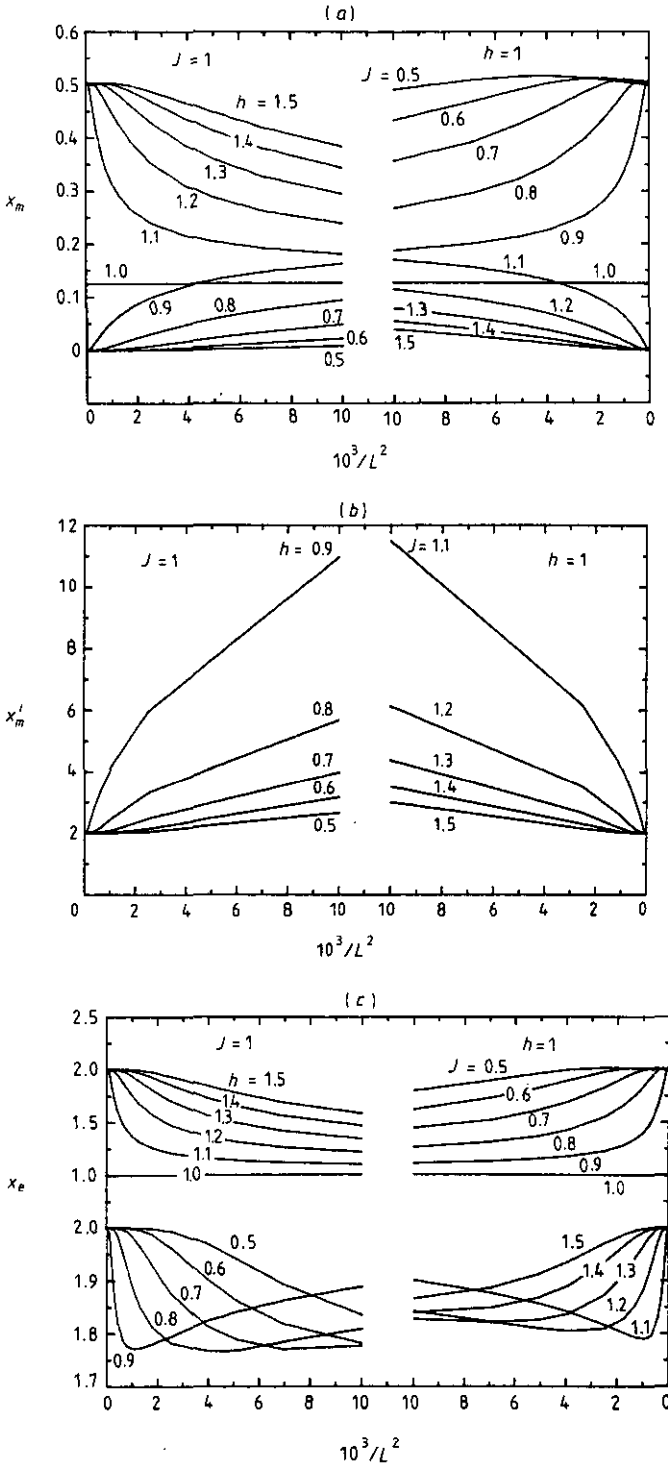


Figure 6. Scaling dimensions deduced from the gap-exponent relations on chains with lengths $L = 10-180$: (a) x_m , (b) x'_m , (c) x_e .

To conclude let us mention that this work is easily extended to the case of a critical sector with an opening angle θ in an otherwise off-critical system.

Note added in proof. The critical behaviour at the interface between two half spaces with different critical temperatures has been recently considered in the framework of wetting theory by Iglói and Indekeu (1990).

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