

Conformal Invariance and Perturbations in the Two-Dimensional Ising Model: Surface Defects

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The influence of homogeneous surface perturbations on the surface critical behavior of the two-dimensional Ising model is studied through finite-size scaling and conformal invariance. Quantum chains of up to 2000 spins are studied in the fermionic version of the model. The results are deduced from the numerical solution of an eigenvalue equation for the excitation spectrum and show that conformal invariance still works for irrelevant surface perturbations.

KEY WORDS: Conformal invariance; Ising models; linear defects; surface properties.

1. INTRODUCTION

Finite-size scaling theory⁽¹⁻³⁾ tells us that in a two-dimensional (2D) system at its critical point in the strip geometry, the correlation length (or inverse gap in the 1D quantum version) associated with an operator diverges like the strip width L . It has been conjectured that the correlation length amplitude is universal⁽⁴⁻⁸⁾ and related in a simple way^(5,6) to the anomalous dimension of the corresponding operator. This remarkable result has since been extensively exploited in the numerical calculations of critical exponents.

Besides the invariance under a uniform change of length scale, it has been suggested⁽⁹⁻¹¹⁾ that under certain restrictions (translational and rotational invariance, short-range interactions) a system at its critical point also may be invariant under local changes of the length scale, i.e., under

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conformal transformations. This property has not been exploited until recently,^(12,13) in particular in 2D problems, where the conformal group is isomorphic with the group of analytic functions.

It was soon realized⁽¹⁴⁾ that finite-size properties at the critical point of 2D systems can be deduced from the known properties of the infinite or semi-infinite systems through a conformal mapping on the strip geometry. The correlation lengths on the strip and their amplitudes are easily obtained, confirming the conjectured results.

Turban⁽¹⁵⁾ suggested that conformal invariance might still hold for the 2D Ising model with a linear defect. This type of perturbation corresponds to a marginal operator⁽¹⁶⁾ leading to a magnetic exponent which is continuously varying with the defect strength.^(17,18) The infinite system with a defect is mapped onto a strip with periodic boundary conditions and two equidistant defect lines. In a numerical study of the 2D classical system⁽¹⁵⁾ the correlation length amplitude was found to vary with the defect strength in the expected way, although the convergence was slow. The amplitude–exponent relation was checked with great accuracy⁽¹⁹⁾ by working with long chains in the fermionic 1D quantum version of the model. The Hamiltonian spectrum was obtained in diagonal form,^(20,21) confirming the validity of conformal invariance for the whole spectrum. An extension to the case of many equidistant defects corresponding to stars of linear defects in the original system has been recently studied.⁽²²⁾

The magnetic exponent of a single line defect on a strip with periodic boundary conditions was previously obtained through finite-size scaling of the defect susceptibility in the case of the 2D Ising universality class, where the defect is marginal, as well as for the 2D q -state Potts model, where the perturbation may be either irrelevant when $q < 2$ or relevant when $q > 2$.⁽²³⁾ A 2D modified Gaussian model with a defect line which may be mapped onto the q -state Potts model and the $O(n)$ model has also been considered in the context of conformal invariance to get the exact q and n dependence of the critical exponents.⁽²⁴⁾

In this work, we consider the case of an irrelevant perturbation in the 2D Ising model. We compare the results of a finite-size scaling study of the thermal and magnetic surface exponents when a surface perturbation is added, with the values deduced from the gap amplitudes when conformal invariance is assumed to remain valid, working on the 1D quantum version of the model.

In Section 2, we present the Hamiltonian of the model, its fermionic version, and the matrices giving the excitation spectrum. In Section 3, we discuss the form of the correlation function, the energy, and the magnetization operators. Section 4 describes the method which is used to get the excitation spectrum of the perturbed system. The results for the thermal

and magnetic exponents obtained through finite-size scaling and conformal invariance are given in Section 5 and discussed in Section 6. The surface magnetization of the perturbed semi-infinite system is calculated in Appendix A and the results of a duality transformation are presented in Appendix B.

2. HAMILTONIAN AND EXCITATION MATRIX

Consider the Ising model in a transverse field h_i with longitudinal coupling J_i on a chain with L spins and free boundary conditions:

$$\mathcal{H} = - \sum_{i=1}^L h_i \sigma_z(i) - \sum_{i=1}^{L-1} J_i \sigma_x(i) \sigma_x(i+1) \quad (2.1)$$

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

$$\sigma_x = \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix}, \quad \sigma_z = \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix} \quad (2.2)$$

\mathcal{H} commutes with the parity operator

$$P = \prod_{i=1}^L \sigma_z(i) \quad (2.3)$$

so that the eigenstates of \mathcal{H} are either even ($P = +1$) or odd ($P = -1$) and may be classified according to their parity.

In the present work we study two types of surface perturbations, either the chain perturbation with

$$\begin{aligned} h_1 &= h_L = h_s \\ h_i &= h, \quad i \neq 1, L \\ J_i &= J \end{aligned} \quad (2.4)$$

or the ladder perturbation, where

$$\begin{aligned} J_1 &= J_{L-1} = J_s \\ J_i &= J, \quad i = 1, \quad L-1 \\ h_i &= h \end{aligned} \quad (2.5)$$

The excitation spectrum of \mathcal{H} may be obtained using standard methods.⁽²⁵⁻²⁷⁾ A Jordan-Wigner transformation

$$c(i) = \prod_{j=1}^{i-1} \exp[i\pi\sigma^+(j)\sigma^-(j)] \sigma^-(i) \quad (2.6a)$$

$$c^+(i) = \sigma^+(i) \prod_{j=1}^{i-1} \exp[-i\pi\sigma^+(j)\sigma^-(j)] \quad (2.6b)$$

yields the fermionic representation

$$\begin{aligned} \mathcal{H} = & - \sum_{i=1}^L h_i [2c^+(i)c(i) - 1] \\ & - \sum_{i=1}^{L-1} J_i [c^+(i) - c(i)][c^+(i+1) + c(i+1)] \end{aligned} \quad (2.7)$$

which is a quadratic form in the fermion operators. It may be diagonalized through the canonical transformation

$$\eta_\alpha = \sum_i [g_{\alpha i}c(i) + h_{\alpha i}c^+(i)] \quad (2.8a)$$

$$\eta_\alpha^+ = \sum_i [g_{\alpha i}c^+(i) + h_{\alpha i}c(i)] \quad (2.8b)$$

leading to

$$\mathcal{H} = E_0 + \sum_\alpha A_\alpha \eta_\alpha^+ \eta_\alpha \quad (2.9)$$

where E_0 is the ground-state energy. The excitations A_α squared are solutions of the eigenvalue equation

$$\bar{A}\bar{\phi}_\alpha = A_\alpha^2 \bar{\phi}_\alpha \quad (2.10)$$

The excitation matrix \bar{A} is the matrix product

$$\bar{A} = (\bar{A} - \bar{B})(\bar{A} + \bar{B}) \quad (2.11)$$

where \bar{A} is symmetric

$$\bar{A} = - \begin{bmatrix} 2h_1 & J_1 & & & & \\ J_1 & 2h_2 & J_2 & & & \\ & J_2 & 2h_3 & \cdot & & \\ & & \cdot & \cdot & \cdot & \\ 0 & & \cdot & 2h_{L-1} & J_{L-1} & \\ & & & J_{L-1} & 2h_L & \end{bmatrix} \quad (2.12a)$$

and $\bar{\bar{B}}$ antisymmetric

$$\bar{\bar{B}} = \begin{bmatrix} 0 & -J_1 & & & & \\ J_1 & 0 & -J_2 & & 0 & \\ & J_2 & 0 & \cdot & & \\ & & \cdot & \cdot & \cdot & \\ 0 & & & \cdot & 0 & -J_{L-1} \\ & & & & J_{L-1} & 0 \end{bmatrix} \tag{2.12b}$$

and such that

$$(\bar{A} + \bar{\bar{B}}) \bar{\phi}_\alpha = A_\alpha \bar{\Psi}_\alpha \tag{2.13a}$$

$$(\bar{A} - \bar{\bar{B}}) \bar{\Psi}_\alpha = A_\alpha \bar{\phi}_\alpha \tag{2.13b}$$

where the normalized eigenvectors $\bar{\phi}$ and $\bar{\Psi}$ are related to the coefficients of the canonical transformation (2.8) through

$$\phi_\alpha(i) = g_{\alpha i} + h_{\alpha i} \tag{2.14a}$$

$$\Psi_\alpha(i) = g_{\alpha i} - h_{\alpha i} \tag{2.14b}$$

In the unperturbed system with $h_s = h$, $J_s = J$, one gets L excitations

$$A_k = 2(h^2 + J^2 + 2hJ \cos k)^{1/2} \tag{2.15}$$

corresponding to standing waves labeled by their quantized wave vectors,

$$k = \frac{(2n + 1) \pi}{2L + 1} \quad (n = 0, 1, \dots, L - 1) \tag{2.16}$$

3. CORRELATION FUNCTION, SURFACE MAGNETIZATION, AND SURFACE ENERGY

For any local operator O_i , the time correlation function reads⁽²⁷⁾

$$G_i(m) = \sum_{\beta \neq 0} |\langle \beta | O_i | 0 \rangle|^2 \exp[-m\tau(E_\beta - E_0)] \tag{3.1}$$

where $|0\rangle$ is the ground state of the system, $|\beta\rangle$ an excited state with energy E_β and τ the infinitesimal imaginary time interval. When $m \rightarrow \infty$ the sum is dominated by the first excited state $|\alpha\rangle$ with nonvanishing matrix element $\langle \alpha | O_i | 0 \rangle$ with the ground state and then

$$\lim_{m \rightarrow \infty} G_i(m) \sim |\langle \alpha | O_i | 0 \rangle|^2 \exp[-m\tau(E_\alpha - E_0)] \tag{3.2}$$

so that the inverse correlation length is proportional to the gap $E_\alpha - E_0$. When $L \rightarrow \infty$, one expects the following scaling behavior for the non-diagonal matrix element at the critical point $h/J = 1$:

$$\langle \alpha | O_i | 0 \rangle \sim L^{-x_0^\alpha} \quad (3.3)$$

where, for free boundary conditions, x_0^α is a surface exponent.

In order to get the anomalous dimensions associated with the surface magnetization and the surface energy, the following matrix elements are convenient:

$$m_s(1) = \langle \sigma | \sigma_x(1) | 0 \rangle \quad (3.4)$$

$$e_s(1) = \langle \varepsilon | \sigma_z(1) | 0 \rangle \quad (3.5)$$

The diagonal terms would be inappropriate: $\langle 0 | \sigma_x(1) | 0 \rangle$ vanishes, since the ground state is even and σ_x anticommutes with the parity operator, whereas $\langle 0 | \sigma_z(1) | 0 \rangle$ contains a disturbing, size-independent regular contribution. In Eq. (3.4), $|\sigma\rangle$ is the lowest eigenstate in the odd sector, since σ_x anticommutes with P and $|\varepsilon\rangle$ in (3.5) is the first excited state in the even sector because σ_z commutes with P .

In the fermionic representation the parity operator reads

$$P = (-1)^L \exp \left[i\pi \sum_{i=1}^L c^+(i) c(i) \right] \quad (3.6)$$

so that when one creates an excitation in the system by acting with η_α^+ on the ground state which is even, the fermion number is changed by one unit and single-particle (or, more generally, odd-particle-number) excited states belong to the odd sector. In the same way, excited states with an even number of particles belong to the even sector. It follows that $|\sigma\rangle$, which is odd, corresponds to the lowest single-particle excited state

$$|\sigma\rangle = \eta_1^+ |0\rangle \quad (3.7a)$$

$$E_\sigma = E_0 + A_1 \quad (3.7b)$$

whereas the two lowest excitations are needed to build $|\varepsilon\rangle$, which is even,

$$|\varepsilon\rangle = \eta_1^+ \eta_2^+ |0\rangle \quad (3.8a)$$

$$E_\varepsilon = E_0 + A_1 + A_2 \quad (3.8b)$$

Putting (3.7a) and (3.8a) into (3.4) and (3.5) and using σ_x and σ_z in the fermion representation, one easily gets

$$m_s(1) = \phi_1(1) \quad (3.9)$$

$$e_s(i) = \Psi_1(i) \phi_2(i) - \Psi_2(i) \phi_1(i) \quad (3.10)$$

$$t_2 = \omega^2 - J_s^2 - 1, \quad s_2 = -h_s J_s \quad (4.7)$$

$$t_{L-1} = \frac{\omega^2 - 2}{J_s}, \quad s_{L-1} = -\frac{1}{J_s} \quad (4.8)$$

$$t_L = \frac{\omega^2 - h_s^2 - J_s^2}{J_s}, \quad s_L = -1 \quad (4.9)$$

The eigenvalues have to satisfy

$$\begin{vmatrix} \psi(L) \\ 0 \end{vmatrix} = \bar{T}_L \bar{T}_{L-1} \bar{T}^{L-4} \bar{T}_2 \bar{T}_1 \begin{vmatrix} 0 \\ 1 \end{vmatrix} \quad (4.10)$$

where $\bar{T} = \bar{T}_i$ ($i = 3$ to $L - 2$).

When $t^2 - 4 < 0$ ($A < 4$), \bar{T} has two complex conjugate eigenvalues

$$\lambda_{\pm} = \theta + i(1 - \theta^2)^{1/2} = e^{\pm i\varphi} \quad (4.11)$$

with $\theta = t/2$, corresponding to propagating modes, whereas when $t^2 - 4 \geq 0$ ($A \geq 4$), the eigenvalues are real

$$\lambda_{\pm} = \theta \pm (\theta^2 - 1)^{1/2} = e^{\pm q} \quad (4.12)$$

and correspond to localized modes.

Let

$$\bar{v}_{\pm} = \begin{vmatrix} 1 \\ \lambda_{\pm} \end{vmatrix}$$

be the eigenvectors; in this basis one may write

$$\bar{T}_2 \bar{T}_1 \begin{vmatrix} 0 \\ 1 \end{vmatrix} = \alpha \bar{v}_+ + \beta \bar{v}_- \quad (4.13)$$

and the second component in Eq. (4.10) leads to the following eigenvalue equation for the propagating modes:

$$(t_L t_{L-1} - J_s)[(\alpha + \beta) \cos(L-3) p + i(\alpha - \beta) \sin(L-3) p] - (t_L/J_s)[(\alpha + \beta) \cos(L-4) p + i(\alpha - \beta) \sin(L-4) p] = 0 \quad (4.14)$$

where

$$\alpha + \beta = t_1 \quad (4.15a)$$

$$i(\alpha - \beta) = \frac{t_1 t_2 - h_s J_s - t_1 \theta}{(1 - \theta^2)^{1/2}} \quad (4.15b)$$

The localized modes are given by

$$(t_L t_{L-1} - J_s)[(\alpha + \beta) \cosh(L-3)q + (\alpha - \beta) \sinh(L-3)q] - (t_L/J_s)[(\alpha + \beta) \cosh(L-4)q + (\alpha - \beta) \sinh(L-4)q] = 0 \quad (4.16)$$

where

$$\alpha + \beta = t_1 \quad (4.17a)$$

$$\alpha - \beta = \frac{t_1 t_2 - h_s J_s - t_1 \theta}{(\theta^2 - 1)^{1/2}} \quad (4.17b)$$

For the chain (ladder) perturbation, one gets L propagating modes when $h_s \leq 1$, $J_s = 1$ ($J_s \geq 1$, $h_s = 1$), whereas two localized modes and $L - 2$ propagating modes are obtained when $h_s > 1$, $J_s = 1$ ($J_s < 1$, $h_s = 1$).

The components of the eigenvectors $\bar{\psi}$ may be deduced from

$$\left| \begin{matrix} \psi(i) \\ \psi(i+1) \end{matrix} \right| = \prod_{j=1}^i \bar{T}_j \left| \begin{matrix} 0 \\ 1 \end{matrix} \right| \quad (4.18)$$

After normalization one gets $\bar{\phi}$ and finally $\bar{\Psi}$ using Eq. (2.13a).

5. MAGNETIC AND THERMAL SURFACE EXPONENTS OF THE CHAIN WITH DEFECTS

The surface magnetization and surface energy have been calculated at the bulk critical point $h = J = 1$ on chains with lengths $L = 10$ to 2000, with either chain or ladder perturbations, using expressions (3.9) and (3.10) for them in terms of the eigenvector components deduced from Eq. (4.18). The results were checked through a tridiagonalization of \mathcal{H} in the spin version for $L \leq 14$ and a diagonalization of \bar{A} for $L \leq 200$.

Since at the critical point

$$m_s(1) \sim L^{-x_m^s} \quad (5.1)$$

$$e_s(1) \sim L^{-x_e^s} \quad (5.2)$$

the surface exponents are given by the slopes of log-log plots and are shown on Figs. 1 and 2 as functions of $1/L^2$.

When $h_s \neq 0$, x_m^s and x_e^s always converge toward the unperturbed surface values^(16,32)

$$x_m^s = 1/2 \quad (5.3)$$

$$x_e^s = 2 \quad (5.4)$$

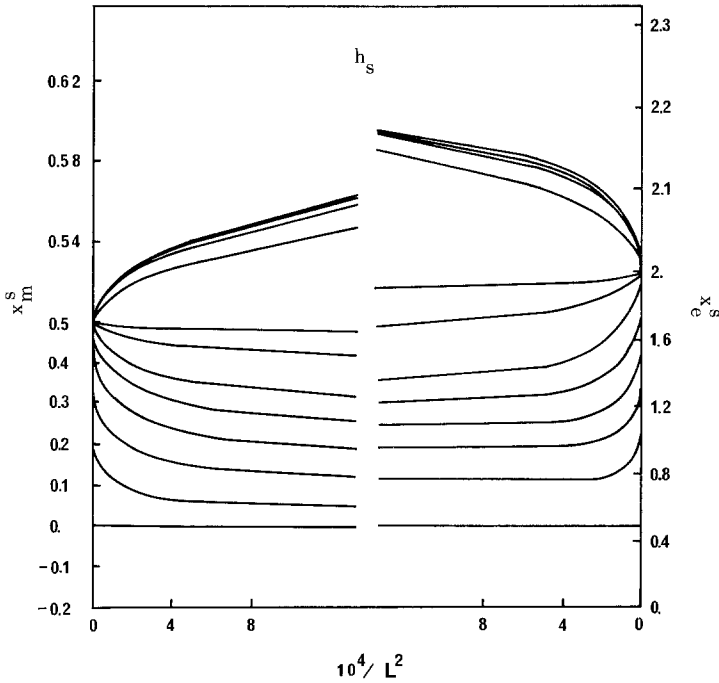


Fig. 1. Critical exponents for the surface magnetization x_m^s and energy x_e^s obtained through finite-size scaling on the Ising chain in a transverse field with size $L = 30$ to 2000 with a surface perturbation $h_s = 5, 4, 3, 2, 1, 0.75, 0.5, 0.4, 0.3, 0.2, 0.1, 1 \times 10^{-5}$ from top to bottom. The method does not allow taking $h_s = 0$, but the same results are obtained with $h_s = 1 \times 10^{-5}$ for the sizes studied.

When $h_s = 0$ these values change to

$$x_m^s = 0 \tag{5.5}$$

$$x_e^s = 1/2 \tag{5.6}$$

The conformal transformation

$$w(z) = (L/\pi) \ln z \tag{5.7}$$

of the complex plane maps the 2D classical semi-infinite system onto a strip with width L and free boundary conditions.⁽¹⁴⁾ This leads to a chain with L spins and free ends in the 1D quantum version. To the algebraic decay of the surface correlation functions at the critical point of the semi-finite system there corresponds an exponential decay on the strip with a correlation length proportional to the strip width and inversely proportional to

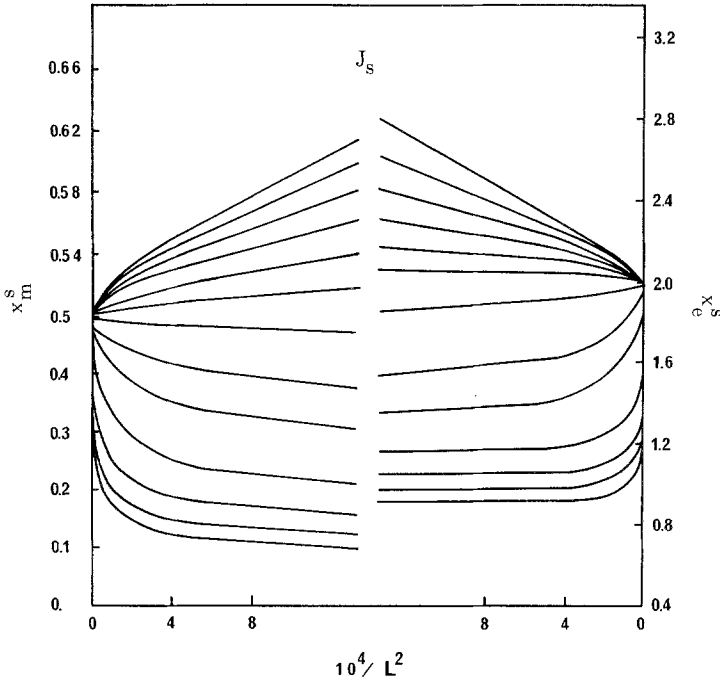


Fig. 2. As on Fig. 1, for a surface perturbation $J_s = 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 1, 1.5, 2, 3, 4, 5, 6$ from top to bottom.

the related surface exponent. In the quantum case on the finite chain, the corresponding gaps vanish like L^{-1} with an amplitude proportional to the surface exponents,⁽¹³⁾

$$G_m = E_\sigma - E_0 = A_1 = \frac{\pi}{L} v_s x_m^s \tag{5.8}$$

$$G_e = E_e - E_0 = A_1 + A_2 = \frac{\pi}{L} v_s x_e^s \tag{5.9}$$

where v_s , the sound velocity, is required on dimensional grounds to relate the gaps with the dimension of an inverse time to the chain length L .⁽³³⁾ It may be deduced from the initial slope of the dispersion relation, which on the finite chain is given by

$$v_s = \frac{\Delta E}{\Delta k} = \frac{L}{\pi} (A_2 - A_1) \tag{5.10}$$

so that, with $E_{v_s} = E_0 + A_2$, the gap of the sound velocity is

$$G_{v_s} = E_{v_s} - E_\sigma = A_2 - A_1 = \frac{\pi}{L} v_s \quad (5.11)$$

The different gaps and excitations are shown on Fig. 3. When Eq. (2.15) is taken at the critical point $h = J = 1$ of the bulk, one gets $A_k = v_s k$ with $v_s = 2$. The correct asymptotic behavior is obtained on the chain with defect using Eq. (5.10) as shown on Fig. 4, except when $h_s = 0$. In this latter case, A_1 vanishes (see Appendix B) and the appropriate gap is

$$G_{v_s} = A_3 - A_2 \quad (5.12)$$

The surface exponents are given by the gap ratios

$$\begin{aligned} x_m^s &= G_m / G_{v_s} \\ x_e^s &= G_e / G_{v_s} \end{aligned} \quad (5.13)$$

and shown on Figs. 5 and 6. A good convergence toward the values given by the finite-size scaling analysis is observed.

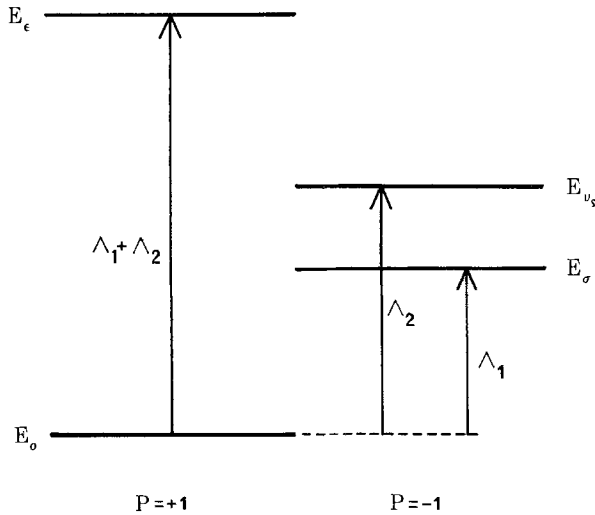


Fig. 3. Energy levels and excitation spectrum in the two parity sectors.

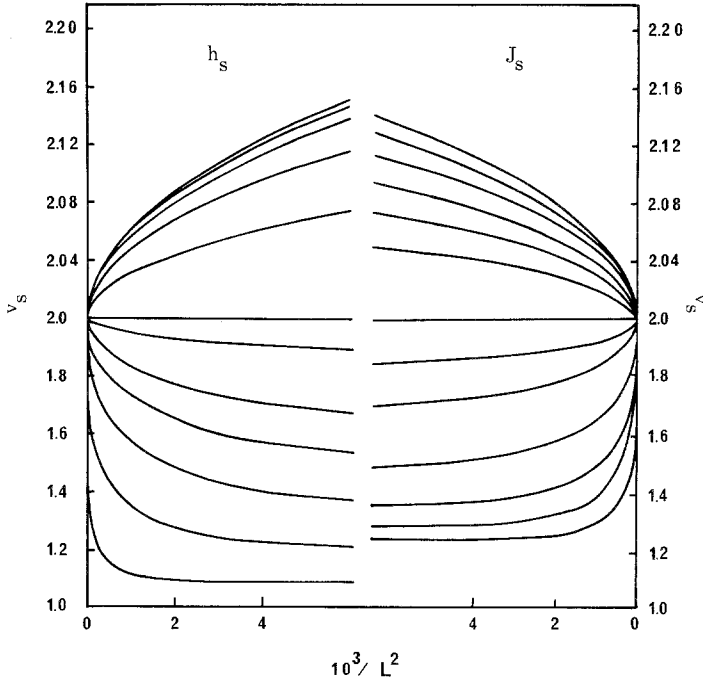


Fig. 4. Sound velocity v_s deduced from the gap $G_{v_s} = A_2 - A_1$ (or $A_3 - A_2$ when $h_s = 0$) for a surface chain perturbation $h_s = 5, 4, 3, 2, 0, 1, 0.75, 0.5, 0.4, 0.3, 0.2, 0.1$ or a surface ladder perturbation $J_s = 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 1, 1.5, 2, 3, 4, 5, 6$ from top to bottom for chain size $L = 10$ to 2000.

6. DISCUSSION

Consider a classical system with a defect where the first-neighbor coupling is perturbed by ΔK so that the change of the internal energy per bond is $\Delta u = \Delta K \langle \sigma_i \sigma_j \rangle = \Delta K \epsilon$. In a scale transformation one gets

$$\Delta u' = b^{d^*} \Delta u \tag{6.1}$$

$$\epsilon' = b^{x_t} \epsilon \tag{6.2}$$

where d^* is the dimension of the defect and x_t is the scaling dimension of the energy operator $\langle \sigma_i \sigma_j \rangle$. The perturbation ΔK scales like

$$\Delta K' = b^{y^*} \Delta K = \Delta u' / \epsilon' = b^{d^* - x_t} \Delta K \tag{6.3}$$

so that its scaling dimension is

$$y^* = d^* - x_t \tag{6.4}$$

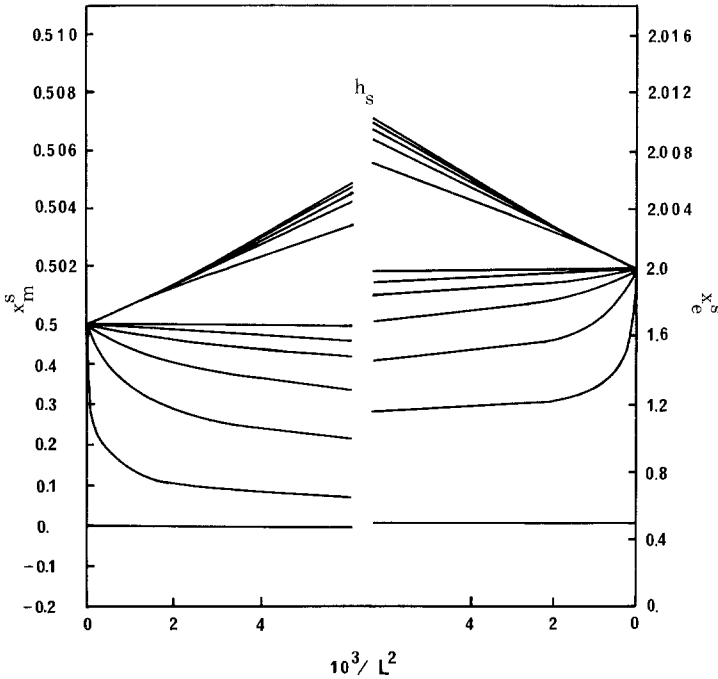


Fig. 5. Critical exponents for the surface magnetization x_m^s and energy x_e^s deduced from the gap ratios G_m/G_{v_s} and G_e/G_{v_s} on the Ising chain in a transverse field with size $L = 10$ to 2000 with a surface perturbation $h_s = 5, 4, 3, 2, 1, 0.75, 0.5, 0.4, 0.3, 0.2, 0.1, 0$ from top to bottom. The values for $h_s = 0$ are obtained via duality on an unperturbed chain with $L - 1$ spins.

In the case of a line perturbation in the bulk of the 2D Ising model where $d^* = x_t = 1$, one gets $y^* = 0$ and the perturbation is marginal. When the perturbation ΔK_s is on the surface of the 2D Ising model, $x_t = x_e^s = 2^{(16,32)}$ and $y^* = y_e^s = 1 - x_e^s = -1$, so that the surface perturbation is irrelevant when ΔK_s is finite. This explains the finite-size scaling results ($x_e^s = 2, x_m^s = 1/2$) for the ladder perturbation when $J_s \neq \infty$ and the chain perturbation when $h_s \neq 0$. The case $h_s = 0$ corresponds to $\Delta K_s = \infty$ in the 2D classical system and then the surface perturbation becomes relevant ($x_e^s = 1/2, x_m^s = 0$). Under renormalization the surface spin remains frozen in the ordered state.

The results deduced from the gaps assuming that conformal invariance is still valid for an irrelevant surface perturbation are not so evident. When the 2D perturbed semi-infinite system is mapped onto a strip by the conformal transformation (5.7) with an inhomogeneous scale factor

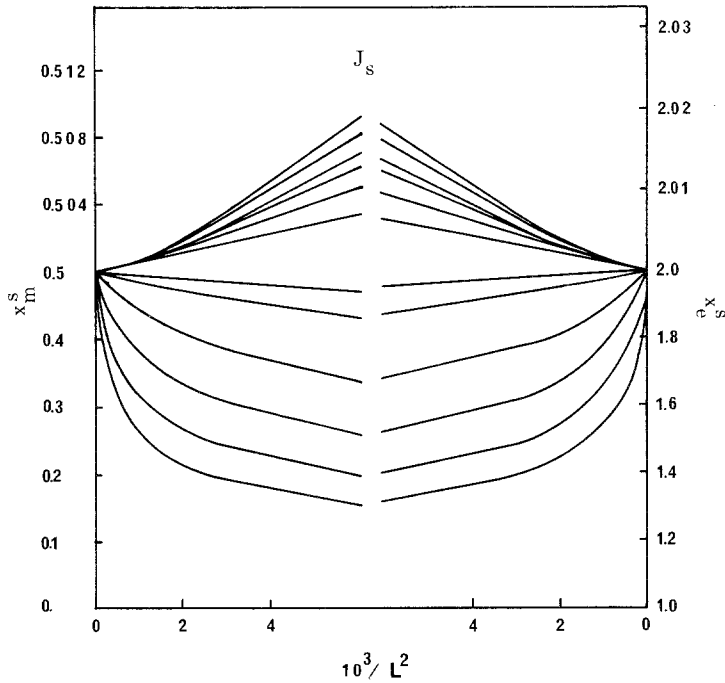


Fig. 6. As on Fig. 5, for a surface perturbation $J_s = 0.7, 0.8, 0.3, 0.9, 0.95, 1, 1.5, 2, 3, 4, 5, 6$ from top to bottom. Notice that at small L the exponents first increase and then decrease with J_s .

$b(z) = |w'(z)|^{-1}$, the irrelevant surface perturbation $\Delta K_s(z) = \Delta K_s$ is rescaled to

$$\Delta K_s(w) = b(z)^{y_s^e} \Delta K_s \tag{6.5}$$

so that we should study the inhomogeneous surface perturbation $\Delta K_s(w)$ on the strip when we use conformal invariance except when $h_s = 0$, since then $\Delta K_s = \infty$ remains unchanged on the strip.

To understand the results obtained for the irrelevant perturbation, we have to suppose that on the semi-infinite system the surface perturbation is already inhomogeneous and given by

$$\Delta K_s(z) = b(z)^{-y_s^e} \Delta K_s \tag{6.6}$$

so that on the strip we recover ΔK_s , the constant surface perturbation which we studied. The validity of conformal invariance implies that the inhomogeneous surface perturbation (6.6) on the semi-infinite system

behaves in the same way as the homogeneous perturbation, i.e., is irrelevant.

Let us now turn to the results obtained with $h_s = 0$. The exponent x_m^s is recovered in an exact calculation of the surface magnetization (Appendix A), leading to

$$m_s(1) = \left| \frac{1 - (h/J)^2}{1 + (h_s/J)^2 - (h/J)^2} \right|^{1/2} \quad (6.7)$$

for the chain defect and

$$m_s(1) = \left| \frac{1 - (h/J)^2}{1 + (h/J_s)^2 - (h/J)^2} \right|^{1/2} \quad (6.8)$$

for the ladder defect when $h/J \leq 1$, so that with $v = 1$, $\beta^s = x_m^s = 1/2$ when $h_s \neq 0$ and $J_s \neq \infty$ and $\beta^s = x_m^s = 0$ when $h_s = 0$ and $J_s = \infty$.

All the results are confirmed by a duality transformation (Appendix B) under which the chain with L spins, free ends, and $h_s = 0$ transforms into an unperturbed chain with $L - 1$ spins, free ends, and a free spin. To $\sigma_z(1)$ corresponds $\mu_x(1)$ on the dual chain and the surface energy of the perturbed system scales like the surface magnetization of the unperturbed one, so that $x_e^s = 1/2$. To $\sigma_x(1)$ corresponds the dual parity operator Q , which is scale invariant and $x_m^s = 0$. This result is recovered if one notices that $\sigma_x(L)$ transforms into $\mu_z(L)$, i.e., the z component of the free spin corresponding to a classical Ising chain at its zero-temperature fixed point. Let us finally mention that to $\sigma_z(i)$ ($i = 2$ to $L - 1$) corresponds the dual operator $\mu_x(i - 1) \mu_x(i)$ with the dimension of a surface energy $x_e^s = 2$, but the surface layer with a slower decay of the correlations gives the leading contribution on the strip.

APPENDIX A. SURFACE MAGNETIZATION OF THE SEMI-INFINITE CHAIN WITH A SURFACE DEFECT

The surface magnetization is given by the amplitude of the normalized eigenvector corresponding to the lowest excitation A_1 on the surface site

$$m_s(1) = \phi_1(1) \quad (A.1)$$

In the semi-infinite system and in the ordered phase ($h/J \leq 1$) the ground-state is degenerate and A_1 vanishes, so that Eq. (2.13a) becomes

$$(\bar{A} + \bar{B}) \bar{\phi}_1 = 0 \quad (A.2)$$

providing a recurrence for $\phi_1(n)$ from which the components of the eigenvector may be deduced

$$\phi_1(2) = -\frac{h_s}{J_s} m_s(1) \tag{A.3}$$

$$\phi_1(n) = \left(\frac{h}{J}\right)^{n-2} \phi_1(2) \tag{A.4}$$

m_s is then determined by the normalization condition⁽³⁰⁾

$$\sum_{n=1}^{\infty} \phi_1^2(n) = 1 = m_s^2(1) \left[1 + \left(\frac{h_s}{J_s}\right)^2 \sum_{p=0}^{\infty} \left(\frac{h}{J}\right)^{2p} \right] \tag{A.5}$$

At the critical point, $h/J = 1$ requires $m_s(1) = 0$, whereas in the ordered phase $h/J < 1$, the geometric serie may be summed, leading to

$$m_s(1) = \left| \frac{1 - (h/J)^2}{1 - (h/J)^2 + (h_s/J_s)^2} \right|^{1/2} \tag{A.6}$$

In the unperturbed system one recovers

$$m_s(1) = [1 - (h/J)^2]^{1/2} \tag{A.7}$$

and $\beta^s = 1/2$. With the surface defect one gets $\beta^s = 1/2$ when $h_s \neq 0$ and $J_s \neq \infty$, and $\beta^s = 0$ when $h_s = 0$ or $J_s = \infty$.

APPENDIX B. DUALITY TRANSFORMATION AND SURFACE CRITICAL BEHAVIOR OF THE CHAIN WITH $h_s = 0$

Let us consider the quantum spin Hamiltonian

$$\mathcal{H} = -h \sum_{i=2}^{L-2} \sigma_z(i) - J \sum_{i=1}^{L-1} \sigma_x(i) \sigma_x(i+1) \tag{B.1}$$

on a chain with free ends, L spins, and vanishing surface field $h_s = 0$. Define the dual spins as

$$\mu_z(i) = \sigma_x(i) \sigma_x(i+1) \quad (1 \leq i < L) \tag{B.2}$$

$$\mu_z(L) = \sigma_x(L) \tag{B.3}$$

$$\mu_x(i) = \prod_{j=1}^i \sigma_z(j) \quad (1 \leq i \leq L) \tag{B.4}$$

and let

$$Q = \prod_{j=1}^L \mu_z(j) \quad (\text{B.5})$$

be the parity operator on the dual chain. The dual operators satisfy the Pauli algebra and lead to the following form for the dual Hamiltonian:

$$\mathcal{H}_D = -h \sum_{i=2}^{L-1} \mu_x(i-1) \mu_x(i) - J \sum_{i=1}^{L-1} \mu_z(i) \quad (\text{B.6})$$

The dual system is an unperturbed chain with $L-1$ spins and free ends together with a free spin $\mu(L)$. It follows that to each state of the chain there correspond the two degenerate states of the free spin and all the levels of \mathcal{H} are at least doubly degenerate. Otherwise stated, the system has a vanishing excitation energy $A_1 = 0$. The surface energy operator $\sigma_z(1)$ on the original system scales like the surface magnetization $\mu_x(1)$ on the dual system and the surface magnetization operators $\sigma_x(1)$ and $\sigma_x(L)$ like the parity operator Q and the free spin energy operator $\mu_z(L)$.

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