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1997 J. Phys. A: Math. Gen. 30 L105

(http://iopscience.iop.org/0305-4470/30/5/006)

J. Phys. A: Math. Gen. **30** (1997) L105–L111. Printed in the UK PII: S0305-4470(97)79365-X

LETTER TO THE EDITOR

Off-diagonal density profiles and conformal invariance

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Received 6 November 1996, in final form 18 December 1996

Abstract. Off-diagonal profiles $\phi_{\rm od}(v)$ of local densities (e.g. order parameter or energy density) are calculated at the bulk critical point, by conformal methods, on a strip with transverse coordinate v, for different types of boundary conditions (free, fixed and mixed). Such profiles, which are defined by the non-vanishing matrix element $\langle 0|\hat{\phi}(v)|\phi\rangle$ of the appropriate operator $\hat{\phi}(v)$ between the ground state and the corresponding lowest excited state of the strip Hamiltonian, enter into the expression of two-point correlation functions on a strip. They are of interest in the finite-size scaling study of bulk and surface critical behaviour since they allow the elimination of regular contributions. The conformal profiles, which are obtained through a conformal transformation of the correlation functions from the half-plane to the strip, are in agreement with the results of a direct calculation, for the energy density of the two-dimensional Ising model.

Following the pioneering work of Fisher and de Gennes [1], the study of order parameter and energy density profiles near surfaces has been an active field of research during the past years. These profiles have been calculated at, and near the critical point, in the mean-field approximation [2], using field-theoretical approaches [3] and through exact solutions [4, 5]. Much progress has also been achieved in their calculation at bulk criticality in two-dimensional (2D) systems making use of conformal techniques [6–12].

In a semi-infinite 2D system, the profile $\phi(y)$ of a fluctuating quantity, such as the order parameter or the energy density, is obtained in the transfer matrix formalism as the diagonal matrix element $\langle 0|\hat{\phi}(y)|0\rangle$ of the corresponding operator $\hat{\phi}$ in the ground state $|0\rangle$ of the Hamiltonian $\mathcal{H} = -\ln \mathcal{T}$, where $\mathcal{T}$ denotes the transfer operator along the surface.

On a strip of infinite length and finite width L, one may also consider the off-diagonal profile $\phi_{\rm od}(v)$, where v is the transverse coordinate. The profile is then defined as the off-diagonal matrix element $\langle 0|\hat{\phi}(v)|\phi\rangle$ between the ground state $|0\rangle$ of the Hamiltonian $\mathcal{H}$ on the strip and its lowest excited state $|\phi\rangle$ leading to a non-vanishing matrix element.

These off-diagonal profiles are commonly used at the bulk critical point to obtain information about the surface and bulk critical behaviour via finite-size scaling, while avoiding the regular terms which contribute to the diagonal ones. Actually, in the absence of an external symmetry-breaking field, an off-diagonal matrix element has to be used to study the scaling behaviour of the order parameter since the diagonal one vanishes, due to symmetry. They are also of interest because of their high degree of universality. One may

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mention two recent studies where off-diagonal profiles are considered at bulk criticality: the spin 1/2–spin 1 Ising quantum chain in [13] and the random Ising quantum chain in [14].

In the following, the scaling form of such off-diagonal matrix elements is obtained at the bulk critical point for 2D conformally invariant systems. It is deduced from the asymptotic behaviour of the appropriate two-point correlation function in the half-space after a conformal transformation to the strip geometry. We consider first symmetric and then asymmetric boundary conditions on the strip and compare our results to some exact expressions of the energy-density profiles, obtained in the appendix, for the Ising model in the extreme anisotropic limit. Since we use conformal methods, non-invariant boundary conditions, like a finite surface field for which an interesting scaling behaviour has been recently observed [15, 16], and off-critical systems are here excluded.

Let us first briefly review the Fisher–de Gennes result and its consequence for the profile on a strip. We consider a non-vanishing profile $\phi(y)$ on a semi-infinite 2D conformally invariant sytem at its critical point with a surface at $y = 0$. It may be the energy density profile with any type of uniform boundary conditions or the order parameter profile with fixed boundary conditions. The problem involves a single length scale, the distance y from the surface. Under a length rescaling by a factor b, the profile transforms as $\phi(y/b) = b^{x_\phi}\phi(y)$ so that

$$\phi(y) = \mathcal{A} y^{-x_\phi} \tag{1}$$

where x_ϕ is the bulk scaling dimension of $\hat{\phi}$. Now, making use of the conformal transformation $w = (L/\pi)\ln z$, with $z = x + \mathrm{i}y = \rho\ \mathrm{e}^{\mathrm{i}\theta}$ and $w = u + \mathrm{i}v$ one obtains

$$\rho = \exp\left(\frac{\pi u}{L}\right) \qquad \theta = \frac{\pi v}{L} \tag{2}$$

and the local dilatation factor is $b(z) = |\mathrm{d}w/\mathrm{d}z|^{-1} = \pi\rho/L$. The half-plane $y > 0$ is transformed into a strip $-\infty < u < +\infty$, $0 < v < L$ with the same boundary conditions as the half-space on both edges [17]. The profile transforms as [18]

$$\phi(w) = b(z)^{x_\phi}\phi(z) \tag{3}$$

so that [6]

$$\phi(v) = \mathcal{A}\left[\frac{L}{\pi}\sin\left(\frac{\pi v}{L}\right)\right]^{-x_\phi}. \tag{4}$$

One may notice that the surface critical behaviour is hidden in the sine variation. At a fixed distance $l \ll L$ from the surface the profile behaves as

$$\phi(l) \simeq \mathcal{A}l\left(1 + \tfrac{1}{6}\pi^2 l^2 x_\phi\, L^{-2} + \cdots\right) \tag{5}$$

in agreement with the Fisher-de Gennes conjecture which gives a L^{-d} correction term [1] with a universal amplitude [9]. Generally, the exponent d is expected to give the scaling dimension x_ϕ^{s} of $\hat{\phi}$ at any surface transition leading to a non-vanishing profile in the semi-infinite critical system [7, 9, 19–21]. The $O(N)$ model at the special transition (for $N < 1$ in 2D) provides a counter-example, the surface energy exponent being smaller than d in this case [12, 22, 23]†.

Let us now turn to the calculation of the off-diagonal matrix element. On the critical semi-infinite system, conformal invariance strongly constrains the form of the connected two-point correlation function, $\mathcal{G}^{\mathrm{con}}_{\phi\phi}(x_1 - x_2, y_1, y_2)$. Applying an infinitesimal special conformal transformation which preserves the surface geometry, one obtains a system of

† We thank E Eisenriegler for pointing out this exception to us.

partial differential equations for $\mathcal{G}_{\phi\phi}^{\text{con}}$, from which the following scaling form is deduced [24]

$$\mathcal{G}_{\phi\phi}^{\text{con}}(x_1 - x_2, y_1, y_2) = (y_1 y_2)^{-x_\phi} g(\omega) \qquad \omega = \frac{(x_1 - x_2)^2 + (y_1 - y_2)^2}{y_1 y_2}. \tag{6}$$

When $\omega \gg 1$, ordinary scaling leads to $g(\omega) \sim \omega^{-x_\phi^{\text{s}}}$ where x_ϕ^{s} is the scaling dimension of $\hat{\phi}$ at the surface. This limit also corresponds to $\rho_1 \gg \rho_2$ where, using polar coordinates, 6 may be rewritten as

$$\mathcal{G}_{\phi\phi}^{\text{con}}(\rho_1, \rho_2, \theta_1, \theta_2) \sim (\rho_1 \rho_2)^{-x_\phi} \left(\frac{\rho_1}{\rho_2}\right)^{-x_\phi^{\text{s}}} (\sin\theta_1 \sin\theta_2)^{x_\phi^{\text{s}} - x_\phi}. \tag{7}$$

We now consider the connected two-point function at bulk criticality in the strip geometry. In the same limit, it can be obtained through the conformal transformation of (7) from the half-plane to the strip geometry with [17]

$$\mathcal{G}_{\phi\phi}(w_1, w_2) = b(z_1)^{x_\phi} b(z_2)^{x_\phi} \mathcal{G}_{\phi\phi}(z_1, z_2) \tag{8}$$

giving:

$$\begin{aligned}\mathcal{G}_{\phi\phi}^{\text{con}}(u_1 - u_2, v_1, v_2) &= \left(\frac{\pi}{L}\right)^{2x_\phi} (\rho_1 \rho_2)^{x_\phi} \mathcal{G}_{\phi\phi}^{\text{con}}(\rho_1, \rho_2, \theta_1, \theta_2) \\ &\sim \left(\frac{\pi}{L}\right)^{2x_\phi} \exp\left[-\frac{\pi x_\phi^{\text{s}}}{L}(u_1 - u_2)\right] \left[\sin\left(\frac{\pi v_1}{L}\right) \sin\left(\frac{\pi v_2}{L}\right)\right]^{x_\phi^{\text{s}} - x_\phi}.\end{aligned} \tag{9}$$

On the strip, making use of the transfer operator $\text{e}^{-\mathcal{H}}$, it can also be written as an expansion over the eigenstates $|n\rangle$ of the critical Hamiltonian $\mathcal{H}$ with eigenvalues E_n and ground state energy E_0

$$\mathcal{G}_{\phi\phi}^{\text{con}}(u_1 - u_2, v_1, v_2) = \sum_{n>0} \langle 0|\hat{\phi}(v_1)|n\rangle \langle n|\hat{\phi}(v_2)|0\rangle \exp[-(E_n - E_0)(u_1 - u_2)]. \tag{10}$$

In the limit $\rho_1 \gg \rho_2$ which corresponds to $u_1 \gg u_2$ on the strip, the sum is dominated by the contribution of the lowest exited state $|\phi\rangle$ with a non-vanishing matrix element so that

$$\mathcal{G}_{\phi\phi}^{\text{con}}(u_1 - u_2, v_1, v_2) \simeq \langle 0|\hat{\phi}(v_1)|\phi\rangle \langle \phi|\hat{\phi}(v_2)|0\rangle \exp[-(E_\phi - E_0)(u_1 - u_2)]. \tag{11}$$

Comparing with (9) we recover the gap-exponent relation $E_\phi - E_0 = \pi x_\phi^{\text{s}}/L$ [17] as a by-product and we may identify the expression of the off-diagonal matrix element

$$\phi_{\text{od}}(v) \sim \left(\frac{L}{\pi}\right)^{-x_\phi} \left[\sin\left(\frac{\pi v}{L}\right)\right]^{x_\phi^{\text{s}} - x_\phi} \tag{12}$$

with symmetric boundary conditions on the strip. The off-diagonal energy-density profile for the Ising model given in equation (A5) of the appendix, which is valid for symmetric free or fixed boundary conditions, agrees with (12) in the continuum limit.

At a fixed distance $l \ll L$ from the surface, $\phi_{\text{od}}(l)$, behaving as $L^{-x_\phi^{\text{s}}}$, is quite appropriate to perform a finite-size scaling study since the regular term which appeared in (5) is now avoided. One may notice that the diagonal profile $\phi(v)$ in (4) is formally recovered with $x_\phi^{\text{s}} = 0$ in (12). Finally, in the half-plane limit ($L \to \infty$), the amplitude of the off-diagonal profile vanishes. This is consistent with the scaling considerations leading to equation (1): a non-vanishing profile on the semi-infinite system necessarily gives the diagonal profile (4) on the strip.

Next we consider the case of mixed boundary conditions on the half-space. This means having different scale-invariant boundary conditions a and b on the positive and negative x-axes, respectively, with $a, b = f$ (free), $+$ or $-$ (fixed). The plane-to-strip conformal transformation leads to different boundary conditions a and b on opposite edges of the strip. The method employed to determine the scaling behaviour of the two-point function in (6) can no longer be used since it supposed translation invariance along the x-direction which is now broken by the mixed boundary conditions on the surface. Fortunately, the two-point correlation functions with mixed boundary conditions have been obtained explicitly for the Ising model using conformal methods [11]: n-point correlation functions in the half-space with mixed boundary conditions are determined by the same differential equation as a particular $2n+2$-point bulk correlation function. Using the results of Burkhardt and Xue [11], when $\rho_1/\rho_2 \gg 1$, the asymptotic spin–spin correlation functions read

$$\begin{aligned}
\mathcal{G}_{\sigma\sigma}^{+-} &\sim (\rho_1\rho_2 \sin\theta_1 \sin\theta_2)^{-1/8}\left[\cos\theta_1\cos\theta_2 + \sin^2\theta_1\sin^2\theta_2\left(\frac{\rho_2}{\rho_1}\right)+\cdots\right]\\
\mathcal{G}_{\sigma\sigma}^{+f} &\sim (\rho_1\rho_2 \sin\theta_1 \sin\theta_2)^{-1/8}(\cos\theta_1\cos\theta_2)^{1/2}\\
&\qquad\times\left[1+\frac{1}{2}\sin\theta_1\sin\theta_2\tan\left(\frac{\theta_1}{2}\right)\tan\left(\frac{\theta_2}{2}\right)\frac{\rho_2}{\rho_1}+\cdots\right]
\end{aligned} \tag{13}$$

whereas the following expressions are obtained for the energy–energy correlation functions

$$\begin{aligned}
\mathcal{G}_{\varepsilon\varepsilon}^{+-} &\sim (\rho_1\rho_2 \sin\theta_1 \sin\theta_2)^{-1}\Big[(1-4\sin^2\theta_1)(1-4\sin^2\theta_2)\\
&\qquad +64\sin^2\theta_1\sin^2\theta_2\cos\theta_1\cos\theta_2\left(\frac{\rho_2}{\rho_1}\right)+\cdots\Big]\\
\mathcal{G}_{\varepsilon\varepsilon}^{+f} &\sim (\rho_1\rho_2 \sin\theta_1 \sin\theta_2)^{-1}\left[\cos\theta_1\cos\theta_2 + 8\sin^2\theta_1\sin^2\theta_2\left(\frac{\rho_2}{\rho_1}\right)+\cdots\right].
\end{aligned} \tag{14}$$

Making use of the conformal transformation to the strip geometry as in the first line of equation (9) and comparing to the expansion of the correlation function on the strip with asymmetric boundary conditions, one may identify the profiles. Since the correlation functions in (13) and (14) are the unconnected ones, the expansion in (10) now contains the term $n=0$. In the limit $u_1-u_2 \gg 1$, the leading contribution is the product of the diagonal profiles $\phi(v_1)\phi(v_2)$, and the next term contains the product of the off-diagonal ones, as before. In this way, one obtains

$$\begin{aligned}
\sigma_{\mathrm{od}}^{+-}(v) &\sim \left(\frac{L}{\pi}\right)^{-1/8}\left[\sin\left(\frac{\pi v}{L}\right)\right]^{15/8}\\
\sigma_{\mathrm{od}}^{+f}(v) &\sim \left(\frac{L}{\pi}\right)^{-1/8}\left[\sin\left(\frac{\pi v}{L}\right)\right]^{7/8}\left[\cos\left(\frac{\pi v}{2L}\right)\right]^{1/2}\tan\left(\frac{\pi v}{2L}\right)\\
\varepsilon_{\mathrm{od}}^{+-}(v) &\sim \left(\frac{L}{\pi}\right)^{-1}\sin\left(\frac{\pi v}{L}\right)\cos\left(\frac{\pi v}{L}\right)\\
\varepsilon_{\mathrm{od}}^{+f}(v) &\sim \left(\frac{L}{\pi}\right)^{-1}\sin\left(\frac{\pi v}{L}\right)
\end{aligned} \tag{15}$$

for the off-diagonal order parameter and energy density profiles. The results of a direct calculation of the off-diagonal energy density profiles, in equations (A6) and (A9) of the appendix, are in agreement with the two last equations of (15) in the continuum limit.

Diagonal profiles on strips with asymmetric boundary conditions for the Ising, Q-state Potts and $O(N)$ models can be found in references [8, 10–12] where they were deduced from the appropriate one-point functions in the half-plane.

With mixed boundary conditions the correction term in ρ_2/ρ_1 gives a first gap vanishing as π/L on the strip: the connection with surface exponents we had before is lost. Contrary to the case of symmetric boundary conditions in equations (4) and (12), there is no simple functional form adapted to the different boundary conditions. The diagonal profiles generally contain a regular leading contribution in their surface finite-size scaling behaviour whereas the off-diagonal ones behave as $L^{-(x_\phi^{\mathrm{s}})_{a,b}}$ with $(x_\sigma^{\mathrm{s}})_{+,-} = (x_\varepsilon^{\mathrm{s}})_{+,-} = (x_\varepsilon^{\mathrm{s}})_f = 2$ and $(x_\sigma^{\mathrm{s}})_f = 1/2$.

One may notice that diagonal and off-diagonal profiles obtained in [14] for the random Ising quantum chain are in quite good agreement with the conformal results given above although the system, which is strongly anisotropic, is *not* conformally invariant. It would be interesting to check whether this is peculiar to the Ising model or if it holds true for other 2D anisotropic systems as well.

We thank H Rieger, M Henkel and D Karevski for helpful discussions and E Eisenriegler for a critical reading of the manuscript. FI is indebted to the Hungarian National Research Fund for financial support under grants no OTKA TO12830, 17485 and 23642.

Appendix

In this appendix, we calculate the off-diagonal energy density profiles on a strip for the Ising model with different boundary conditions. We work in the extreme anisotropic limit [25] where the critical Hamiltonian reads

$$\mathcal{H} = -\frac{1}{2}\left[\sum_{j=1}^{L-1}\sigma_x(j)\sigma_x(j+1) + \sum_{j=2}^{L-1}\sigma_z(j) + h_1\sigma_z(1) + h_L\sigma_z(L)\right] \qquad \text{(A1)}$$

where $\sigma_x(j)$ and $\sigma_z(j)$ are Pauli matrices at site j. The diagonization proceeds in two steps [26, 27]: first the Hamiltonian is rewritten as a quadratic form in fermion operators, $c^\dagger(j)$ and $c(j)$, using the Jordan–Wigner transformation [28] and then it is diagonalized through a canonical transformation to new fermion operators, $\eta_k^\dagger$ and η_k, such that

$$\begin{aligned} c(j) &= \frac{1}{2}\left\{\sum_k [\varphi_k(j)+\psi_k(j)]\eta_k + [\varphi_k(j)-\psi_k(j)]\eta_k^\dagger\right\} \\ c^\dagger(j) &= \frac{1}{2}\left\{\sum_k [\varphi_k(j)+\psi_k(j)]\eta_k^\dagger + [\varphi_k(j)-\psi_k(j)]\eta_k\right\}. \end{aligned} \qquad \text{(A2)}$$

φ_k and ψ_k are normalized eigenvectors, which are conveniently calculated by a diagonalization process, as described in [29].

With free boundary conditions, $h_1 = h_L = 1$, the eigenvectors are given by

$$\begin{aligned} \varphi_k(j) &= (-1)^j \frac{2}{\sqrt{2L+1}} \cos\left[\frac{2k-1}{2L+1}\left(\frac{j-1}{2}\right)\pi\right] \\ \psi_k(j) &= (-1)^{j+1} \frac{2}{\sqrt{2L+1}} \sin\left(\frac{2k-1}{2L+1} j\pi\right) \end{aligned} \qquad \text{(A3)}$$

with $k = 1, 2, \ldots, L$. The off-diagonal energy density profile is expressed as

$$\varepsilon_{\mathrm{od}}^{ff}(j) = \langle 0|\sigma_z(j)|\varepsilon\rangle = 2\langle 0|c^\dagger(j)c(j)|\varepsilon\rangle \qquad \text{(A4)}$$

where the ground state $|0\rangle$ is the fermion vacuum and $|\varepsilon\rangle$ is the lowest eigenstate with two fermionic excitations so that one obtains

$$\begin{aligned}\varepsilon_{\rm od}^{ff}(j) &= \varphi_1(j)\psi_2(j) - \varphi_2(j)\psi_1(j)\\ &= \frac{4}{2L+1}\left\{\sin\left(\frac{\pi}{2L+1}\right)\cos\left[\frac{4(j+1/2)\pi}{2L+1}\right] - \cos\left(\frac{\pi}{2L+1}\right)\right.\\ &\quad\left.\times\ \sin\left[\frac{(2j-1/2)\pi}{2L+1}\right]\right\}. \end{aligned} \tag{A5}$$

When $L \gg 1$, the first term may be neglected and the second one gives the off-diagonal profile in equation (12) since, for the 2D Ising model, $x_\varepsilon = 1$ and $x_\varepsilon^{\rm s} = 2$ at the ordinary surface transition.

When the two boundary spins are fixed one has to put $h_1 = h_L = 0$ and then the Hamiltonian in equation (A1) describes both the $++$ and the $+-$ boundary conditions. Instead of solving this problem explicitly one may use the duality properties of the quantum Ising model [25]. Through a duality transformation, the critical system with $++$ $(+-)$ boundary condition is related to the energy (magnetization) sector of the critical free chain†, with the correspondence $L \to L-1$ and $j \to j-1$. Then the $\varepsilon_{\rm od}^{++}(j)$ energy density profile is directly given by (A5) with the above substitutions.

To calculate the $+-$ profile one considers the magnetization sector of the free chain, where the two lowest states are $\eta_1^\dagger|0\rangle$ and $\eta_2^\dagger|0\rangle$. Then the $\varepsilon_{\rm od}^{+-}(j)$ profile is given by

$$\begin{aligned}\varepsilon_{\rm od}^{+-}(j) &= \varphi_1(j)\psi_2(j) + \varphi_2(j)\psi_1(j)\\ &= \frac{16}{2L-1}\cos\left[\frac{(2j-1)\pi}{4L-2}\right]\sin\left[\frac{(j-1)\pi}{2L-1}\right]\left\{\cos^2\left[\frac{(2j-1)\pi}{4L-2}\right]-\sin^2\left[\frac{(j-1)\pi}{2L-1}\right]\right\}.\end{aligned} \tag{A6}$$

which asymptotically behaves as $\varepsilon_{\rm od}^{+-}(j) \approx 2\sin(2j\pi/L)/L$ in agreement with the conformal result in (15).

The $+f$ boundary condition is realized with a vanishing transverse field $h_1 = 0$ on the first spin. Then $\sigma_x(1)$ commutes with $\mathcal{H}$ and remains fixed in one of its eigenstates corresponding to $\sigma_x(1) = \pm 1$. This introduces a vanishing excitation in the system which doubles the spectrum. The behaviour of the zero-mode eigenvectors is anomalous:

$$\varphi_0(j) = 0 \qquad \psi_0(j) = (-1)^{j+1}\sqrt{\frac{1}{L}}. \tag{A7}$$

The next fermion state is characterized by the eigenvectors

$$\begin{aligned}\varphi_1(j) &= (-1)^j\sqrt{\frac{2}{L}}\sin\left[\frac{(j-1)\pi}{L}\right]\\ \psi_1(j) &= (-1)^{j+1}\sqrt{\frac{2}{L}}\cos\left[\frac{(j-1/2)\pi}{L}\right].\end{aligned} \tag{A8}$$

In terms of eigenvectors the profile is similar to (A5) and, due to the vanishing of $\varphi_0(j)$, it takes the form

$$\varepsilon_{\rm od}^{+f}(j) = -\varphi_1(j)\psi_0(j) = \frac{\sqrt{2}}{L}\sin\left[\frac{(j-1)\pi}{L}\right] \tag{A9}$$

in agreement with (15) in the continuum limit.

The results in equations (A5), (A6) and (A9) have been checked numerically on small-size quantum Ising chains.

† The energy (magnetization) sector corresponds to an even (odd) number of fermion excitations in the system.

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