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Structure function, susceptibility and correlation lengths at critical points for infinite strips with periodic boundary conditions

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Abstract. We employ the results of conformal invariance at critical points to calculate the structure function $S(\boldsymbol{k})$, bulk susceptibility χ and correlation lengths (defined via moments of the correlation function) for infinite strips with periodic boundaries. Analytic formulae for operators with anomalous dimension $0 \leqslant x \leqslant 1$ are obtained. The correction to the leading asymptotic form of S for large $|\boldsymbol{k}|$ is determined. The convergence to the leading $1/k^{2-2x}$ behaviour is shown to depend on x and be slow for $x=\frac{1}{8}$, the Ising spin-spin correlation function value. For $x=1$, S is found to display a logarithmic lineshape.

By use of the conformal invariance of critical correlation functions (Polyakov 1970), Cardy (1984) has determined the two-point correlation function in an infinite strip of width L with periodic boundary conditions

$$g(y, \theta)=\frac{(2\pi/L)^{2x}}{[2\cosh(2\pi y/L)-2\cos(2\pi\theta/L)]^{x}}. \tag{1}$$

In (1) the separation of the two points along the strip is $y \equiv y_1 - y_2$, while $\theta \equiv \theta_1 - \theta_2$ refers to the separation *across* the strip. In the formulae that follow (except (2)-(5)) we set $L=2\pi$ for simplicity. Results for general L may be obtained by use of (1) and the definition of the quantity of interest, or equivalently by use of standard scaling relations.

Equation (1) is normalised so that $g \to 1/r^{2x}$ for $r \to 0$, where r is the distance between the points. Note that as $y \to \infty$

$$g \to \exp[-x(2\pi/L)y] \tag{2}$$

so that the corresponding correlation length (defined via the asymptotic behaviour of g) is

$$\xi_y^{(a)}=(1/2\pi x)L \tag{3}$$

(Cardy 1984).

In this paper we report results for the structure function (scattering function, when g is the order parameter-order parameter correlation function) which we define as the

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Fourier transform of (1) per unit area. Here the two points (θ_1, y_1) and (θ_2, y_2) must each be integrated over the strip in the transform, since each (θ_1, y_1) or (θ_2, y_2) value arises from the scattering amplitude from a scatterer at that location. Thus

$$S(k_y, k_\theta) \equiv \frac{1}{L}\int_{-\infty}^{+\infty} \mathrm{d}y \int_{-L}^{L} \mathrm{d}\theta \left(1-\frac{|\theta|}{L}\right) g(y, \theta) \exp[\mathrm{i}(k_y y + k_\theta \theta)]. \tag{4}$$

The separate integration of θ_1 and θ_2 over a finite region gives rise to the term with $|\theta|$ in (4) and additionally limits the range of θ values included. Hence, the full periodicity of g in θ is not used and we have a Fourier integral rather than a Fourier series. Of course our results for $S(k_y, k_\theta)$ coincide with the Fourier series coefficients at corresponding k_θ values.

The evaluation of (4) is carried out below. The (bulk) susceptibility χ (integral of the correlation function per unit area) is simply $S(0)$. The correlation lengths, defined as moments via

$$\xi_y^{(\mathrm{m})^2} = \frac{1}{2} \frac{\iint (1-|\theta|/L)(y^2) g(y, \theta)\, \mathrm{d}y\, \mathrm{d}\theta}{\iint (1-|\theta|/L) g\, \mathrm{d}y\, \mathrm{d}\theta} \tag{5}$$

(and similarly for $\xi_\theta^{(\mathrm{m})}$ by replacing y^2 by θ^2) may then be obtained by direct integration or from the second derivatives of S at $\boldsymbol{k}=0$. The reason for the factor of $\frac{1}{2}$ on the RHS of (5) will become clear on comparison of $\xi_y^{(\mathrm{a})}$ and $\xi_y^{(\mathrm{m})}$.

Using (1) and the identity

$$A^{-x} = \frac{1}{\Gamma(x)} \int_0^\infty \exp(-uA) u^{x-1}\, \mathrm{d}u \tag{6}$$

in (4), S becomes a weighted integral over u of a k_y dependent factor

$$f(k_y) = 2K_{\mathrm{i}k_y}(2u) \tag{7}$$

and a k_θ dependent factor

$$h(k_\theta) = \alpha(k_\theta) I_0(2u) + \sum_{k=1}^{\infty} I_k(2u) \beta(k, k_\theta) \tag{8}$$

where K and I are modified Bessel functions. The coefficients in (8) are expressible as

$$\alpha(k_\theta) = 2\pi \left(\frac{\sin \pi k_\theta}{\pi k_\theta}\right)^2 \tag{9}$$

$$\beta(k, k_\theta) = \frac{4}{\pi} \frac{k^2 + k_\theta^2}{(k^2 - k_\theta^2)^2} \sin^2 \pi k_\theta. \tag{10}$$

On integration over u one finally obtains (for strips of width 2π)

$$S(k_y, k_\theta) = \frac{\Gamma(1-x)}{2\Gamma(x)} \left(\alpha(k_\theta) \left| \frac{\Gamma(x/2 + \mathrm{i}k_y/2)}{\Gamma(1-(x+\mathrm{i}k_y)/2)} \right|^2 + \sum_{k=1}^{\infty} \beta(k, k_\theta) \left| \frac{\Gamma((x+k+\mathrm{i}k_y)/2)}{\Gamma(1-(x-k+\mathrm{i}k_y)/2)} \right|^2 \right). \tag{11}$$

It should be noted that the correlation function g, as given by (1), is only determined up to a non-universal multiplicative constant. The same factor affects the structure function and susceptibility but not the correlation lengths, since in this latter case it is divided out (see equation (5)).

It follows from (11) that the bulk susceptibility in an infinite strip of width 2π is

$$\chi = S(0) = \pi \frac{\Gamma^2(x/2)\Gamma(1-x)}{\Gamma^2(1-x/2)\Gamma(x)} = -\frac{4\pi}{x}\frac{B(x/2, x/2)}{B(-x/2, -x/2)} \tag{12}$$

where B is the beta function (Abramowitz and Stegun 1964). It is straightforward to expand χ for small x or small $\varepsilon \equiv 1-x$

$$\begin{aligned}\chi &= (4\pi/x)(1+\tfrac{1}{2}\zeta(3)x^3+\tfrac{3}{8}\zeta(5)x^5+O(x^6))\\ &= (4\pi/x)(1+0.601x^3+0.389x^5+O(x^6))\end{aligned} \tag{13}$$

$$\begin{aligned}\chi &= (\pi/\varepsilon)[1+4(\ln 2)\varepsilon+8(\ln^2 2)\varepsilon^2+(\tfrac{4}{3}\lambda(3)-\tfrac{2}{3}\zeta(3)+\tfrac{32}{3}\ln^3 2)\varepsilon^3+O(\varepsilon^4)]\\ &= (\pi/\varepsilon)(1+2.7726\varepsilon+3.8436\varepsilon^2+4.1533\varepsilon^3+O(\varepsilon^4))\end{aligned} \tag{14}$$

where ζ denotes the zeta function and λ is defined in Abramowitz and Stegun (1964). These results are illustrated in figure 1.

The divergence of χ as $x \to 1$ arises from the short distance behaviour of $g \sim 1/r^2$. This only occurs in the continuum limit; the integral will be cut off at r approximately equal to the lattice spacing for any physical system. The value of the cutoff is not determined by the conformal theory.

As $x \to 0$, conversely, χ diverges due to the diverging range of g in the y direction (cf equation (3)). It is noteworthy that for the Ising spin operator ($x=\frac{1}{8}$) χ is given by the leading term (in equation (13)) to within 0.12% (Cardy 1985). This occurs because the correlation function g for such small x values is essentially one dimensional.

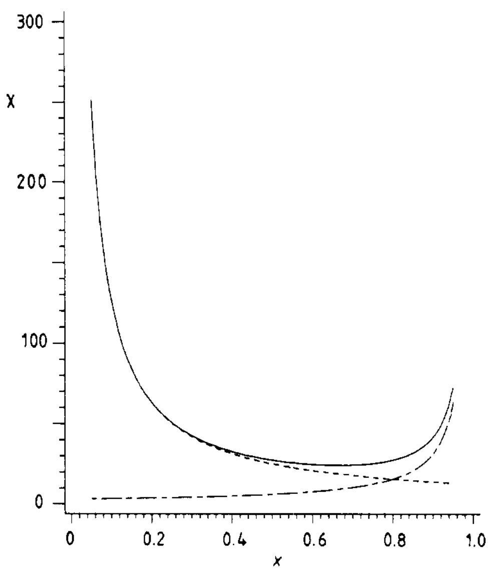

Figure 1. Bulk susceptibility (integral of the order parameter-order parameter correlation function per unit area) χ for an infinite strip of width 2π with periodic boundary conditions plotted against anomalous dimension x. Full curve: conformal result (equation (12)). Broken curve: leading behaviour as $x \to 0$ ($\chi = 4\pi/x$, equation (13)). Chain curve: leading behaviour as $x \to 1$ ($\chi = \pi/(1-x)$, equation (14)). Results for strips of width L follow from ordinary scaling, $\chi(L) = \chi(2\pi)(L/2\pi)^{2-2x}$, $0 \leq x \leq 1$. χ is only determined up to a non-universal multiplicative constant (see text).

The correlations lengths were determined for strips of width 2π as explained above with the result

$$\xi_y^{(m)} = \tfrac{1}{2}(\psi'(x/2) - \psi'(1-x/2))^{1/2} \tag{15}$$

where ψ is the digamma function. Privman and Redner (1985) report a closely related quantity for self-avoiding walks: We also found

$$\xi_\theta^{(m)} = \left[\frac{\pi^2}{3} - \sum_{v=1}^{\infty} 2\left(\frac{B(-x/2, v/2)}{B(x/2, v/2)}\frac{x}{v(v-x)}\right)^2\right]^{1/2}. \tag{16}$$

For $x \to 0$ or $\varepsilon = 1 - x \to 0$, we obtain

$$\begin{aligned}\xi_y^{(m)} &= (1/x)[1 - \tfrac{1}{4}\zeta(3)x^3 - \tfrac{1}{8}\zeta(5)x^5 + O(x^6)] \\ &= (1/x)(1 - 0.3005x^3 - 0.1296x^5 + O(x^6))\end{aligned} \tag{17}$$

$$\begin{aligned}\xi_y^{(m)} &= (\tfrac{7}{2}\zeta(3)\varepsilon)^{1/2}\left(1 + \frac{31\zeta(5)}{28\zeta(3)}\varepsilon^2 + O(\varepsilon^3)\right) \\ &= 2.901\varepsilon^{1/2}(1 + 0.9551\varepsilon^2 + O(\varepsilon^3))\end{aligned} \tag{18}$$

$$\xi_\theta^{(m)} = (\pi/\sqrt{3})(1 - \tfrac{1}{30}\pi^2 x^2 + O(x^3)). \tag{19}$$

For $\varepsilon \to 0$, $\xi_\theta^{(m)}$ vanishes as $\varepsilon^{1/2}$. These results are shown in figure 2 along with $\xi_y^{(a)}$ (equation (3)) for comparison. Note that $\xi_{y,\theta}^{(m)}$ vanish as $x \to 1$ due to the divergence of χ which appears in the denominator of (5). The factor of $\frac{1}{2}$ in the definition of $\xi^{(m)}$ (equation (5)) may now be justified by $\xi_y^{(m)} \to \xi_y^{(a)}$ as $x \to 0$. For the one-dimensional function $g = e^{-cy}$, the two correlation lengths coincide exactly. For the Ising spin case ($x = \frac{1}{8}$) they differ by only 0.06%, consistent with our result for χ.

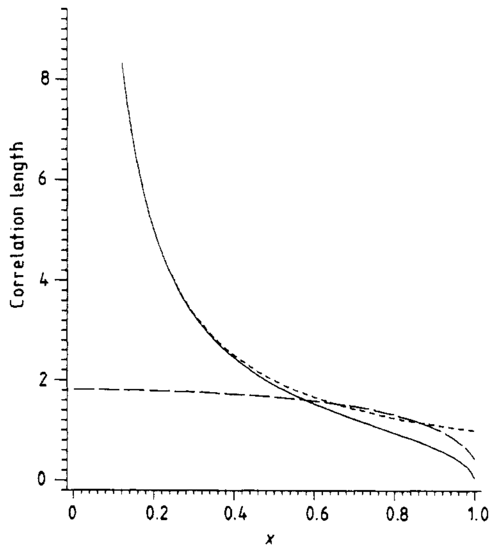

Figure 2. Correlation lengths for an infinite strip of width 2 with periodic boundary conditions plotted against anomalous dimension x. Full curve: correlation length in the long (y) direction $\xi_y^{(m)}$ defined as a moment (equation (5)). Dotted curve: correlation length in the long direction defined via the asymptotic value of the correlation function, $\xi_y^{(a)} = 1/x$ (equation (3)). Broken curve: moment correlation length in the short (θ) direction $\xi_\theta^{(m)}$. For strips of width L, $\xi(L) = \xi(2\pi)(L/2\pi)$.

Finally, we discuss the behaviour of $S(\boldsymbol{k})$, again for strips of width 2π. For $x \to 0$, one has

$$S(k_y, k_\theta) = \frac{2x}{x^2 + k_y^2}[A + (2\gamma A + B)x + O(x^2)] \tag{20}$$

where γ is Euler's constant and

$$A = \alpha(k_\theta) + \sum_{k=1}^{\infty} \beta(k, k_\theta) \frac{k_y^2}{k^2 + k_y^2}$$

$$B = 2\alpha(k_\theta) \operatorname{Re} \psi\left(\mathrm{i}\frac{k_y}{2}\right) + \sum_{k=1}^{\infty} \beta(k, k_\theta) \frac{k_y^2}{k^2 + k_y^2}\left[1 + 2 \operatorname{Re} \psi\left(\frac{k + \mathrm{i}k_y}{2}\right) + 2\frac{k}{k^2 + k_y^2}\right]. \tag{21}$$

Note that for $k_\theta = 0$, one has $A = 2\pi$, $B = 4\pi \operatorname{Re} \psi(\mathrm{i}ky/2)$ and

$$S = \frac{4\pi x}{x^2 + k_y^2}\{1 + 2[\gamma + \operatorname{Re} \psi(\mathrm{i}k_y/2)]x + O(x^2)\}. \tag{22}$$

As $x \to 0$, (20) reduces to

$$S(k_y, k_\theta) = 4\delta(k_y) \sin^2 \pi k_\theta / k_\theta^2 \tag{23}$$

due to the one-dimensional behaviour of g in this limit.

For 'intermediate' values of x, $0 < x < 1$, S exhibits a pronounced maximum at $k = 0$ with subsidiary peaks located at $k_y = 0$ and $k_\theta = \pm\frac{3}{2}, \pm\frac{5}{2}, \ldots$, with heights that decrease with $|k_\theta|$. These features are due to the periodicity of g in the θ coordinate. As x increases, the half-width of the maximum at $\boldsymbol{k} = 0$ in the y direction follows the trend of the (inverse) behaviour of the corresponding correlation length $\xi_y^{(\mathrm{m})}$. The half-width in the θ direction also increases as x increases from 0, but more slowly. At $x \simeq 0.6$ the two half-widths are approximately equal. The subsidiary maxima also broaden much more rapidly in the k_y direction than the k_θ direction as x increases.

The behaviour of S as $|\boldsymbol{k}| \to \infty$ may also be determined. From (11) one finds, for $k_\theta = 0$ and $|k_y| \to \infty$,

$$S = \pi \frac{\Gamma(1-x)}{\Gamma(x)}\left(\frac{k_y}{2}\right)^{2(x-1)}\left(1 + \frac{x(x-1)(x-2)}{3} k_y^{-2} + O(k_y^{-4})\right) \tag{24}$$

while for $k_y = 0$ and $k_\theta = \pm$integer, $|k_\theta| \to \infty$,

$$S = \pi \frac{\Gamma(1-x)}{\Gamma(x)}\left(\frac{k_\theta}{2}\right)^{2(x-1)}\left(1 - \frac{x(x-1)(x-2)}{3} k_\theta^{-2} + O(k_\theta^{-4})\right). \tag{25}$$

Note that the convergence to the asymptotic large k form, $S \sim k^{2(x-1)} = 1/k^{2-\eta}$ depends on the anomalous dimension x. For $x = \frac{1}{8}$ (appropriate to the Ising spin–spin correlation function) the second term in (24) or (25) is less than 1% of the leading one only when $|k| > 16/L$ for a strip of width L. This slow convergence with k has also been observed for scattering functions for Ising models in fully finite systems with free boundary conditions (Kleban *et al* 1986a, b) and in infinite systems at $T \neq T_\mathrm{c}$ with fixed $k\xi$, where ξ is the bulk correlation length (Tracy and McCoy 1975). It also follows from (24) and (25) that the leading asymptotic form is achieved at considerably smaller $|k|$ values when x is close to 1 or 0. In this context, it should be remembered that for any real system, the conformal results which hold in the continuum limit will be cut off for $|k| \gtrsim 1/a$, $a =$ lattice spacing, due to short distance corrections. However, this high

k cutoff will be independent of the strip width L, in contrast to the k value governing the onset of the leading term in (24) or (25), which will scale as $1/L$.

As $\varepsilon = 1 - x \to 0$, (11) gives

$$S(k_y, k_\theta) = \frac{\pi}{\varepsilon}\left\{1 - \left[2\gamma + \frac{\alpha(k_\theta)}{\pi}\,\mathrm{Re}\,\psi\left(\frac{1+\mathrm{i}k_y}{2}\right) + \sum_{k=1}^{\infty}\frac{\beta(k,k_\theta)}{\pi}\,\mathrm{Re}\,\psi\left(\frac{1+k+\mathrm{i}k_y}{2}\right)\right]\varepsilon + \mathrm{O}(\varepsilon^2)\right\} \tag{26}$$

so that the Fourier transform in (4) diverges as $1/\varepsilon$, due to the short-distance behaviour of g. This feature is unphysical for the reasons given above. It may be remedied by defining, for $x < 1$,

$$\tilde{S}(\boldsymbol{k}) = S(\boldsymbol{k}) - S(0) \tag{27}$$

which is equivalent to replacing the exponential in (4) by $\exp[\mathrm{i}(k_y y + k_\theta\theta)] - 1$.

This redefinition does not affect the lineshape of the structure function since the divergent term in (26) is independent of $\boldsymbol{k}$. It follows that, as $x \to 1$, $\tilde{S}(\boldsymbol{k})$ is determined by the $\mathrm{O}(\varepsilon)$ term in the curly bracket in (26). This function is illustrated in figure 3. For $k_y \to \infty$, k_θ fixed,

$$\tilde{S} \to 2\pi\psi(\tfrac{1}{2}) - \alpha(k_\theta)\ln\tfrac{1}{2}k_y - \sum_{k=1}^{\infty}\frac{\beta(k,k_\theta)}{2}\ln\{[(1+k)^2 + k_y^2]/4\}. \tag{28}$$

It is easy to see that S is bounded above and below by $f(k_\theta)\ln|k_y| + C(k_\theta)$ in this limit. If k_θ is an integer,

$$\tilde{S} \to -2\pi(\gamma + \ln 2) - \pi\ln[(1+k_\theta)^2 + k_y^2] \tag{29}$$

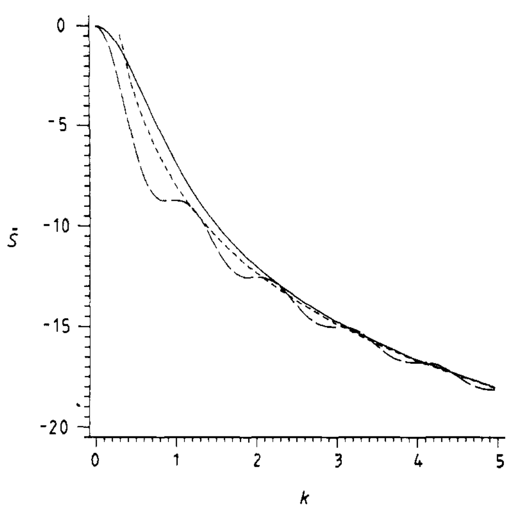

Figure 3. Subtracted structure function $\tilde{S}$ (see equation (27)) for an infinite strip of width 2π with periodic boundary conditions and anomalous dimension $x = 1$. Full curve: $\tilde{S}$ against k_y for $k_\theta = 0$. The $|k_y| \to \infty$ behaviour is logarithmic as per equation (29). For $k_y = 0$, the dotted curve gives the form of $\tilde{S}$ valid for $|k_\theta| \to \infty$, $|k_\theta| =$ integer (equation (31)) while the broken curve illustrates the exact value (equation (30)). Negative values for $\tilde{S}$ are due to its definition (equation (27)). The lineshape is not altered by this feature (see text).

as $k_y \to \infty$. For $k_y = 0$

$$\tilde{S}(k_\theta) = -\sum_{k=1}^{\infty}\sum_{n=1}^{\infty} \beta(k, k_\theta)\frac{1}{n}\left(\frac{2k}{n+k} - \frac{k}{2n+k}\right) \tag{30}$$

which, for k_θ an integer, behaves as

$$\tilde{S} \to -2\pi(\gamma + \ln 2) - 2\pi \ln|k_\theta| \tag{31}$$

as $|k_\theta| \to \infty$. Thus $\tilde{S}$ has a logarithmic lineshape at large k_y or k_θ. This feature is due to the $1/r^2$ behaviour of g at small distances.

The structure function satisfies $S(\boldsymbol{k}) \geqslant 0$ since it is the Fourier transform of a two-point correlation function. Negative values of $\tilde{S}$ and the approach of $\tilde{S}$ to $-\infty$ at large $|k|$ for $x = 1$ are, on the other hand, permissible since an infinite term has been subtracted in defining this quantity (equation (27)).

Finally, we note that recent transfer matrix calculations (Bartelt and Einstein 1986) on the simple Ising model agree well with our results. For $T = T_c$ and infinite cylinders of circumference L, $6 \leqslant L/a \leqslant 9$, $S(k_y)$ (with $k_\theta = 0$) agrees with (11) within 5% or better for $0 \leqslant k_y \leqslant 1$. For larger k values, the structure functions at different widths are not related by scaling, presumably due to non-universal short-distance effects. Note that the k range of agreement, for these L values, is below the point at which the leading asymptotic term in S is dominant (see the discussion following equation (25)).

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