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LETTER TO THE EDITOR

Finite-size scaling and the two-dimensional XY model

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Abstract. We show that the finite-size scaling assumption, and particularly a conjectured relation involving the exponent η, are valid in the low-temperature phase of the 2D XY model, order by order in a perturbative expansion of the two-point correlation function.

1. Introduction

The finite-size scaling hypothesis was first formulated by Fisher (1972). It has been used in various domains of statistical mechanics, in order to extrapolate to the thermodynamical limit results concerning finite systems (Monte Carlo method) or systems which are infinite in only one dimension (transfer matrix method). The latter procedure has mostly been applied to 2D systems: the partially infinite systems are then strips of width N. This method, introduced by Nightingale (1976) for the Ising model, was generalised to various models: self-avoiding walk (Derrida 1981), percolation (Derrida and Vannimenus 1980, Kinzel and Yeomans 1981), O(2)–Heisenberg (or XY) model (Hamer and Barber 1981), Anderson localisation problem (Pichard and Sarma 1981), roughening transition (Luck 1981a, b), etc. These last three cases exhibit an infinite-order Kosterlitz–Thouless transition, and possess a whole line of fixed points.

The general framework of finite-size scaling was shown to be valid in every dimension $d<4$ for ϕ^4-type theories (Brézin 1982). Our aim is to show that the same scaling behaviours hold for $d=2$ along the 'gaussian fixed line', i.e. for a continuous infinity of critical points.

2. The model

We use the XY model, defined by the action

$$S=-\frac{1}{T}\sum_{\langle i,j\rangle}[\cos(\theta_i-\theta_j)-1] \tag{1}$$

where the sum runs over nearest-neighbour pairs of sites on a 2D square lattice; the spacing a is equal to unity.

Kosterlitz and Thouless (1973; Kosterlitz 1974) proved that the region $0\leqslant T\leqslant T_c$ corresponds to the 'gaussian fixed line' mentioned above.

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We consider the two-point correlation function

$$\Gamma(L) = \langle \exp \mathrm{i}(\theta_0 - \theta_L)\rangle \tag{2}$$

in the following two geometries:

(A) *infinite 2D lattice*: (2) will be denoted $\Gamma_\infty(L)$;

(B) *strip of finite width N* (we consider only longitudinal correlations: the vector $\boldsymbol{L}$ is parallel to the direction of infinite length): (2) will be denoted $\Gamma_N(L)$

Let us recall the results for (2) in the case of the Ising model at $T = T_c$. The expressions given in Nightingale (1976) lead easily to

$$\begin{aligned} &\Gamma_N(L) \sim \exp(-L/\xi_N) \qquad \text{with } \xi_N = aN, \\ &\Gamma_\infty(L) \sim L^{-\eta}, \end{aligned} \tag{3}$$

where the values of a and η are

$$a = 4/\pi, \qquad \eta = \tfrac{1}{4}. \tag{4}$$

3. Low-temperature expansion

We introduce the Fourier transform

$$\theta_p = \sum_r \theta(\boldsymbol{r})\, \mathrm{e}^{-\mathrm{i}pr} \leftrightarrow \theta(\boldsymbol{r}) = \int \widetilde{\mathrm{d}p}\; \mathrm{e}^{\mathrm{i}pr}\theta_p.$$

The measure in momentum space depends on the geometry:

$$\text{(A)} \int \widetilde{\mathrm{d}p} = \int_{-\pi}^{+\pi} \frac{\mathrm{d}p_1}{2\pi} \int_{-\pi}^{+\pi} \frac{\mathrm{d}p_2}{2\pi},$$

$$\text{(B)} \int \widetilde{\mathrm{d}p} = \frac{1}{N}\sum_n \int_{-\pi}^{+\pi} \frac{\mathrm{d}p_2}{2\pi} \qquad \text{with } p_1 = 2\pi\frac{n}{N}.$$

The power series expansion of the cosine, and a field rescaling $\varphi = T^{-1/2}\theta$, lead to a bare propagator

$$\pi(\boldsymbol{p}) = \langle \varphi_p \varphi_{-p}\rangle = \Big(2\sum_\mu (1 - \cos p_\mu)\Big)^{-1} \tag{5}$$

and to interaction terms

$$\begin{aligned} -S_M = \frac{T^{M-2/2}}{M!} \int \widetilde{\mathrm{d}p}_1 \ldots \widetilde{\mathrm{d}p}_M \varphi_{p_1} \ldots \varphi_{p_M} (2\pi)^2\, \delta(\boldsymbol{p}_1 + \ldots + \boldsymbol{p}_M) \\ \times \sum_\mu \Big(2 \sin \frac{p_1^\mu}{2}\Big) \ldots \Big(2 \sin \frac{p_M^\mu}{2}\Big) \end{aligned} \tag{6}$$

where $M = 4, 6, 8, \ldots$ is an arbitrary even integer.

The calculation of (2) is equivalent to the introduction of the following source term:

$$-\delta S = \mathrm{i}[\theta(\boldsymbol{0}) - \theta(\boldsymbol{L})] = \mathrm{i}T^{1/2} \int \widetilde{\mathrm{d}p}\; \varphi_p[1 - \exp(-\mathrm{i}p_2 L)]. \tag{7}$$

The quantity $\ln \Gamma(L)$ is the sum of all connected graphs with a non-zero even number of sources.

4. Leading-order results

The lowest-order contribution is equal to the free field graph g_0 (figure 1)

$$\ln \Gamma^{(0)}(L) = -\frac{T}{2}\int \widetilde{\mathrm{d}p}\frac{1-\cos p_2 L}{\Sigma_\mu (1-\cos p_\mu)}. \tag{8}$$

In the following, $\ln\Gamma(L)$ will denote *the divergent part* of (2) as $L\to\infty$, and the superscript (0) means: in leading-order approximation.

Figure 1. The leading-order (free field) contribution to the two-point function.

The infrared divergences of (8) depend on the geometry: in the case (A), the propagator can be replaced by $1/p^2$, which leads to

$$\ln \Gamma^{(0)}_\infty(L) = -(T/2\pi)\ln L; \tag{9}$$

in the case (B), the only term to contribute is the one corresponding to $p_1 = 0$,

$$\ln \Gamma^{(0)}_N(L) = -TL/2N. \tag{10}$$

These results are analogous to those of the Ising model (3), with

$$a^{(0)} = 2/T \qquad \text{and} \qquad \eta^{(0)} = T/2\pi.$$

When L and N are both large and comparable, we have a scaling behaviour interpolating between (9) and (10): let us consider the quantity

$$\psi(L,N) = -\frac{2}{T}\ln\Gamma^{(0)}_N(L) = \frac{1}{N}\sum_n \int_{-\pi}^{\pi}\frac{\mathrm{d}p_2}{2\pi}\frac{1-\cos p_2 L}{\Sigma_\mu (1-\cos p_\mu)}.$$

Integration over p_2 leads to

$$\psi(L,N) = \frac{1}{N}\sum_{1\leqslant n\leqslant N}\frac{1-\mathrm{e}^{-LX_n}}{\sinh X_n}$$

with $\sinh X_n/2 = \sin \pi n/N$, or $\cosh X_n + \cos 2\pi n/N = 2$.

This sum can be rearranged in the form

$$\psi(L,N) = L/N + \Sigma_1 + \Sigma_2 + \Sigma_3,$$

where

(i) $$\Sigma_1 = \frac{2}{N}\sum_{1\leqslant n\leqslant N/2}\left(\frac{1}{\sinh X_n} - \frac{N}{2\pi n}\right)$$

has a finite limit when N goes to infinity:

$$\Sigma_1 \to I = \frac{1}{\pi}\int_0^{\pi/2}\mathrm{d}\theta\left(\frac{1}{\sin\theta(1+\sin^2\theta)^{1/2}} - \frac{1}{\theta}\right) = -\frac{1}{\pi}\ln\frac{\pi}{2\sqrt{2}}.$$

(ii) $$\Sigma_2 = \frac{1}{\pi}\sum_{1\leqslant n\leqslant N/2}\frac{1}{n} = \frac{1}{\pi}\left[\ln\frac{N}{2} + \gamma + \mathrm{O}\left(\frac{1}{N}\right)\right]$$

(γ is Euler's constant).

(iii) $$\Sigma_3 = -\frac{2}{N} \sum_{1 \leqslant n \leqslant N/2} \frac{e^{-LX_n}}{\sinh X_n}$$

is dominated by the lowest values of n, where we have

$$X_n = 2\pi \frac{n}{N} + O(1/N^3)$$

and then

$$\Sigma_2 = (1/\pi) \ln[1 - \exp(-2\pi L/N)] + O(1/N^2).$$

We have obtained the scaling behaviour

$$\psi(L, N) = (1/\pi) \ln N + \varphi(L/N) + O(1/N)$$

with (11)

$$\varphi(x) = \frac{1}{\pi} \ln\left(\frac{2\sqrt{2}\, e^{\gamma}}{\pi} \sinh 2\pi x\right).$$

The expansions of φ around $x = 0$ and $x = \infty$ give respectively (9) and (10) again.

5. Higher orders

In order to study the infrared divergences of a general graph, let us investigate first the integrations on internal lines. Let $\boldsymbol{k}$ be the momentum of one of them (figure 2).

12148 **Figure 2.** A typical internal line.
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The corresponding integrand is

$$\sin \tfrac{1}{2}k^{\mu} \cdot \sin \tfrac{1}{2}k^{\nu} \Big/ \sum_{\rho} \sin^2 \tfrac{1}{2}k^{\rho}.$$

This quantity is always less than unity (in absolute value). The measure on the Brillouin zone being normalised, we can therefore deduce the following:

(1) no divergence is due to internal lines;

(2) the limit of a (B) graph when N tends to infinity is equal to the corresponding (A) graph, by obvious continuity reasons.

We are only left with star-like graphs, as represented in figure 3. Their contribution reads

$$g(M) = (-1)^{M/2} \frac{T^{M-1}}{M!} \int \prod_i \widetilde{\mathrm{d}k}_i (2\pi)^2 \, \delta^2\left(\sum_i \boldsymbol{k}_i\right) \prod_i [1 - \exp(-\mathrm{i}k_{i,2}L)]$$

$$\times \prod_i \frac{1}{2\sum_{\mu_i}(1 - \cos k_{i,\mu_i})} \sum_{\nu} \prod_i 2 \sin \frac{k_{i,\nu}}{2}.$$

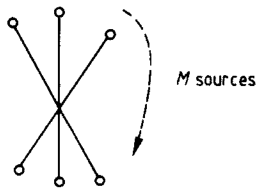
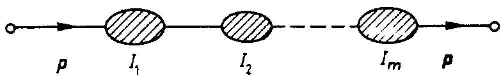


Figure 3. The general star-like graph, with M external sources and no loop.

(3) These integrals are manifestly UV convergent.

(4) Their infrared behaviour is obtained by usual power counting: their superficial IR convergence degree is $\delta_M = M-2$.

We can conclude that the divergent part of (2) is entirely given by the graphs with two external sources. Their general shape is given in figure 4.



12152 **Figure 4.** The general shape of IR divergent graphs.

Let $I_K(\mathbf{0})_{\mu\nu}$ be the value of the Kth irreducible subgraph I_K at zero (external) momentum, for given external indices μ and ν. Symmetry implies

$$I_K(\mathbf{0})_{\mu\nu} = \delta_{\mu\nu} I_K(\mathbf{0}).$$

We have then

$$g = \int \widetilde{\mathrm{d}p} \frac{2(1-\cos p_2 L)}{[\sum_\nu 2(1-\cos p_\nu)]^{m+1}} [I_1(\mathbf{0}) \ldots I_m(\mathbf{0}) + \mathrm{O}(p^2)] \sum_{\{\mu\}} \prod_i \left(-4\sin^2 \frac{p_i, \mu_i}{2}\right).$$

All propagators disappear, except one of them, and we find

$$g = \prod_{I \subset g} (-I(\mathbf{0})) g_0 \tag{12}$$

where g_0 is the lowest-order result (8) and the I's are all irreducible sugraphs of g.

Resummation of (12) is formally very simple. Let $f(T)$ be the power series

$$f(T) = -\sum_I I(\mathbf{0}) \tag{13}$$

where the sum runs over all irreducible graphs. Then we obtain

$$\ln \Gamma_N(L) = (1-f(T))^{-1} \ln \Gamma_N^{(0)}(L). \tag{14}$$

We conclude from the above discussion that the divergent part of the correlation function factorises:

one factor is the free-field (or gaussian) result (9)–(11),

the other is a temperature renormalisation.

As a consequence of this very simple formula, we have proved (to all orders in T) that

$$\Gamma_N(L) \sim \exp(-L/aN), \qquad \Gamma_\infty(L) \sim L^{-\eta},$$

where a and η depend on a single function f:

$$a(T)=2[1-f(T)]/T, \qquad \eta(T)=T/2\pi[1-f(T)]. \tag{15}$$

The product of these quantities is then constant:

$$a\eta=1/\pi. \tag{16}$$

This relation which is also true for the Ising model at $T=T_c$ (see (4)), has been conjectured to be valid for several 2D models: percolation and the Potts model (Derrida and De Sèze 1982), and was used to extract the exponent $\eta(T)$ from strip-method data in localisation (Pichard and Sarma 1981) and surface roughening (Luck 1981a, b) problems.

6. Expansion up to T^3 and value of T_c

The graphs which contribute to the function $f(T)$ up to order T are given in figure 5.

A large number of these low-order graphs can be evaluated by means of symmetry properties: for example, let us consider the only one-loop graph g_1,

$$g_1=-\frac{T}{2}\int \widetilde{\mathrm{d}k}\frac{-4\sin^2\frac{1}{2}k_1}{\Sigma_\mu 4\sin^2\frac{1}{2}k_\mu}.$$

The similar integral corresponding to the second component would of course be equal to g_1, which implies that $g_1=T/4$.

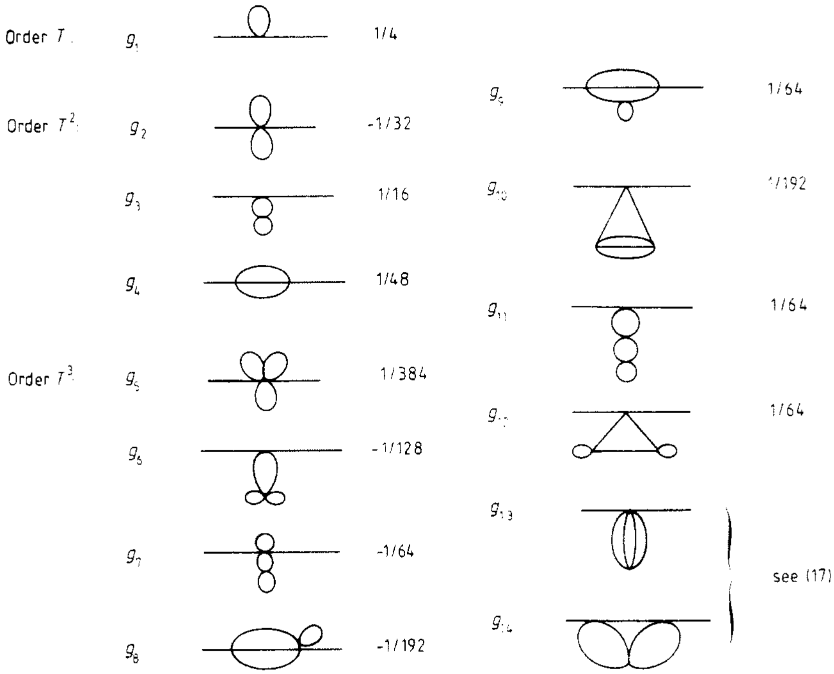


Figure 5. All graphs contributing to the temperature-renormalisation function $f(T)$ up to order T^3.

Analogous symmetry considerations enable us to compute all graphs shown in figure 5, except g_{13} and g_{14}. The contributions of these last two ones were computed in configuration space. We had to evaluate lattice sums of two functions φ and ψ related to the propagator $a\,(\boldsymbol{x})$:

$$\begin{aligned} g_{13} &= -\frac{T^3}{24}\sum_{\boldsymbol{x}}[\varphi^4(x)+\psi^4(x)] = -\frac{T^3}{24}\gamma_{13}, \\ g_{14} &= \frac{T^3}{4}\sum_{\boldsymbol{x},\boldsymbol{y}}[\varphi^2(\boldsymbol{x})+\psi^2(\boldsymbol{x})][\varphi^2(\boldsymbol{y})+\psi^2(\boldsymbol{y})]\varphi(\boldsymbol{x}-\boldsymbol{y}) = \frac{T^3}{4}\gamma_{14}, \end{aligned} \tag{17}$$

with

$$\varphi(\boldsymbol{x}) = -\tfrac{1}{4}[2a(\boldsymbol{x})-a(\boldsymbol{x}+\boldsymbol{1})-a(\boldsymbol{x}-\boldsymbol{1})],$$

$$\psi(\boldsymbol{x}) = -\tfrac{1}{4}[a(\boldsymbol{x}+\boldsymbol{1}-\boldsymbol{2})-a(\boldsymbol{x}+\boldsymbol{1})-a(\boldsymbol{x}-\boldsymbol{2})+a(\boldsymbol{x})].$$

The propagator $a(\boldsymbol{x})$ can be constructed by means of explicit recursion relations, as explained in Spitzer (1976).

The sums in (17) are very rapidly converging towards the numbers

$$\gamma_{13} = 0.068\,309\,8662, \qquad \gamma_{14} = 0.043\,727\,2207.$$

The resulting expansion of $f(T)$ is then

$$f(T) = \tfrac{1}{4}T + \tfrac{5}{96}T^2 + f_3T^3 + \mathrm{O}(T^4) \tag{18}$$

with

$$f_3 = 0.034\,127\,2266.$$

In order to test this expansion, we looked for the value of T_c in the following manner. We know from Kosterlitz and Thouless (1973) and Kosterlitz (1974) that η has an algebraic singularity at $T = T_c$:

$$\eta(T) \approx \tfrac{1}{4} - \alpha(T_c - T)^{1/2}. \tag{19}$$

We then expanded the quantity $(\frac{1}{4}-\eta)^2$ in powers of T, using (15) and (18), and determined the first real zero of the polynomial.

We give the values $T_c^{(n)}$ obtained by a truncation of $f(T)$ at order T^n:

$$T_c^0 = 0.7854, \qquad T_c^{(1)} = 0.8328, \qquad T_c^{(2)} = 0.8655, \qquad T_c^{(3)} = 0.8785. \tag{20}$$

These numbers converge rather well towards a value of $T_c \approx 0.90$, to be compared with the best estimate we know: $T_c = 0.900 \pm 0.006$, based on the high-temperature expansion (Betts *et al* 1971).

7. Conclusion

We proved that the scale invariant low-temperature phase of the XY model is described by one single T-renormalisation function f. This implies that the scaling of correlations (11), and in particular the relation (16), are valid in the whole phase $T \leqslant T_c$. This approach is also quantitatively correct (20), but any extrapolation of so short an expansion needs some amount of added information (19).

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