

On the role of Fourier modes in finite-size scaling above the upper critical dimension

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Renormalization-group theory stands, since over 40 years, as one of the pillars of modern physics. As such, there should be no remaining doubt regarding its validity. However, finite-size scaling, which derives from it, has long been poorly understood above the upper critical dimension d_c in models with free boundary conditions. Besides its fundamental significance for scaling theories, the issue is important at a practical level because finite-size, statistical-physics systems, with free boundaries above d_c , are experimentally accessible with long-range interactions. Here we address the roles played by Fourier modes for such systems and show that the current phenomenological picture is not supported for all thermodynamic observables either with free or periodic boundaries. Instead, the correct picture emerges from a sector of the renormalization group hitherto considered unphysical.

In this Letter we address a subtle question, still open in the theory of finite-size scaling (FSS). Although it may cursorily appear an academic exercise, this question has to be decisively and convincingly resolved since it concerns the very foundations of the renormalization group (RG), one of the greatest achievements of theoretical physics [1]. Given the nature of our investigation, and with the aim of a comprehensive presentation, we emphasize essential historical and relatively technical elements of the theory before introducing the problem of Fourier modes in the treatment of boundary conditions.

FSS is a well developed component of modern theories of critical phenomena. It was initially introduced on heuristic grounds [2] and then understood within the frame of Wilson's RG [1, 3–5]. The system's inverse typical linear scale L^{-1} appears like the reduced temperature $t = (T - T_c)/T_c$ or magnetic field $h = H/T_c$ as a scaling field governing flow towards the RG fixed points (FP)

which control the critical singularities of thermodynamic properties,

$$C(t) \sim |t|^{-\alpha}, \quad m(t) \underset{t \leq 0}{\sim} |t|^\beta, \quad m(h) \sim |h|^{1/\delta}, \quad (1)$$

$$\chi(t) \sim |t|^{-\gamma}, \quad \xi(t) \sim |t|^{-\nu}, \quad g(\mathbf{x}) \sim |\mathbf{x}|^{-(d-2+\eta)}. \quad (2)$$

Here, C , m , χ , ξ and g are, respectively, the singular parts of the specific heat, magnetization, susceptibility, correlation length and correlation function, and the fields t or h when not specified are zero. The long-distance properties at the FP's depend on space dimension d and order-parameter symmetry, but not on details such as the short range of microscopic interactions, or lattice symmetry. Hence, there exists a set of properties (the critical exponents as well as combinations of critical amplitudes, not considered here) which *rigorously* take the same values for different systems. Magnetic systems, for example, can share these properties with fluids. This is the meaning of the term “universality” used in this context [6].

The usual phenomenological argument for FSS (which turns out to be valid only below the upper critical dimension) can be summarized as follows [2, 5]. Assume a quantity P exhibits a singularity in the vicinity of the critical point T_c , measured by a critical exponent ρ , so that $P(t) \sim |t|^\rho$. Then, the singularity develops in a finite-size system as

$$P(t, L^{-1}) \sim P(t, 0) [L/\xi(t)]^{-\frac{\rho}{\nu}}, \quad (3)$$

where, it is argued, the ratio $L/\xi(t)$ appears because it involves the only two length scales governing long-distance behavior, and the power on the right-hand side is such that the singularity in t is washed out at T_c for the finite system. This argument predicts a FSS exponent γ/ν for the susceptibility, and $-\beta/\nu$ for the magnetization.

A spectacular result of Wilson's RG is the explanation for the existence of an upper critical dimension d_c above which Landau mean-field theory (MFT) is recovered, with

$$\alpha = 0, \quad \beta = 1/2, \quad \delta = 3, \quad (4)$$

$$\gamma = 1, \quad \nu = 1/2, \quad \eta = 0 \quad (5)$$

for ϕ^4 -field theory. To fix ideas, let us consider a nearest-neighbour Ising model consisting of spins $s_{\mathbf{x}}$ located on the sites $\mathbf{x}$ of a regular hypercubic lattice with unit vectors $\boldsymbol{\mu}$ ($|\boldsymbol{\mu}| = a$, the lattice spacing). The exact partition function

$$Z = \sum_{\{s_{\mathbf{x}}\}} \exp \left[\beta \left(J \sum_{\mathbf{x}} \sum_{\boldsymbol{\mu}} s_{\mathbf{x}} s_{\mathbf{x}+\boldsymbol{\mu}} + H \sum_{\mathbf{x}} s_{\mathbf{x}} \right) \right] \quad (6)$$

can be rewritten via a Hubbard-Stratonovich transformation as a functional integral over $\phi(\mathbf{x}) \in \mathbb{R}$, $Z \simeq \prod_{\mathbf{x}} \int d\phi(\mathbf{x}) e^{-S[\phi]}$, with

$$S[\phi] = \int d^d x \left(f_0 + \frac{r_0}{2} \phi^2 + \frac{u}{4} \phi^4 + \frac{c}{2} |\nabla \phi|^2 - h \phi \right), \quad (7)$$

where $f_0 = -a^{-d} \ln 2$, $r_0 = a^{-2} t$, $u = 2a^{d-4}$, $c = (2d)^{-1}$ and $h = \beta a^{-(d/2+1)} H$. Dimensional analysis shows that the free energy f_0 has scaling dimension d , the coefficient r_0 , proportional to the reduced temperature, has dimension $y_t = 2$, the coefficient of the quartic term u has $y_u = 4 - d$ and the magnetic field has $y_h = d/2 + 1$. The eigenvalues $y_i > 0$ control the flow of the relevant fields at the FP, leading to homogeneity:

$$f(t, h) = b^{-d} F(b^{y_t} t, b^{y_h} h), \quad (8)$$

$$\xi(t, h) = b \Xi(b^{y_t} t, b^{y_h} h), \quad (9)$$

$$g(t, h, \mathbf{x}) = b^{-d+2} G(b^{y_t} t, b^{y_h} h, b^{-1} \mathbf{x}). \quad (10)$$

The critical exponents in Eqs. (1)-(2) emerge through the scaling laws,

$$\alpha = (2y_t - d)/y_t, \quad \beta = (d - y_h)/y_t, \quad \delta = y_h/(d - y_h), \quad (11)$$

$$\gamma = (2y_h - d)/y_t, \quad \nu = 1/y_t, \quad \eta = d - 2y_h + 2. \quad (12)$$

Above $d_c = 4$, $y_u < 0$, and one expects that critical behavior should be controlled by the Gaussian FP $(t, h, u) = (0, 0, 0)$. But a discrepancy between the MFT exponents in Eqs. (4) and Eqs. (11) indicates that the limit $u \rightarrow 0$ has to be taken with care; u is a *dangerous irrelevant variable* (DIV) [7], at least, as was first thought, in the free-energy sector. The agreement between Eqs. (5) and (12) suggests that there is no danger in the sector of the correlations [8]. A proper inclusion of this mechanism resolves the discrepancy in the free-energy sector. In Fourier space, for a periodic system, the quadratic part of the action (7) reads $\frac{1}{2} \sum_{\mathbf{k}} (|\mathbf{k}|^2 + r_0) |\phi_{\mathbf{k}}|^2$, and the quartic term $\frac{1}{4} u \int d^d x \phi^4(\mathbf{x}) = \frac{u}{4L^d} \sum_{\mathbf{k}_1 \mathbf{k}_2 \mathbf{k}_3} \phi_{\mathbf{k}_1} \phi_{\mathbf{k}_2} \phi_{\mathbf{k}_3} \phi_{-\mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3}$ can be expanded as $\frac{1}{4} \frac{u}{L^d} \phi_0^4 + \frac{3}{2} \frac{u}{L^d} \phi_0^2 \sum_{\mathbf{k}} |\phi_{\mathbf{k}}|^2$ up to higher-order corrections in the non-zero modes, such that the action can be approximated by

$$S[\phi] \simeq \frac{1}{2} \left(r_0 + \frac{3u}{2L^d} \sum_{\mathbf{k} \neq 0} |\phi_{\mathbf{k}}|^2 \right) \phi_0^2 + \frac{u}{4L^d} \phi_0^4 + \frac{1}{2} \sum_{\mathbf{k} \neq 0} (r_0 + c|\mathbf{k}|^2) |\phi_{\mathbf{k}}|^2 - h L^{d/2} \phi_0. \quad (13)$$

Only the zero mode couples to h and its quartic self-interaction means that u is dangerous. The non-zero modes neither couple to h nor have a dangerous quartic term.

The zero mode is thus responsible for anomalous FSS behavior above d_c and leads to

$$f(t, u, h) = b^{-d} F \left(\frac{b^{y_t} t - b^{y_u} u}{b^{y_u/2} u^{1/2}}, \frac{b^{y_h} h}{b^{y_u/4} u^{1/4}} \right). \quad (14)$$

The temperature field t is governed by a modified RG exponent $y_t^* = y_t - \frac{1}{2}y_u = \frac{d}{2}$ and the magnetic field h by $y_h^* = y_h - \frac{1}{4}y_u = \frac{3d}{4}$ [9–11]. Temperature dependencies of the magnetization and susceptibility follow by differentiating (14) wrt h and choosing the scale factor $b = (t/u^{1/2})^{-2/d}$. Hence

$$m(t, u, 0) = B(u)t^{1/2}M \left[1 - A(u)t^{1-4/d} \right], \quad (15)$$

$$\chi(t, u, 0) = \Gamma(u)t^{-1}X \left[1 - A(u)t^{1-4/d} \right] \quad (16)$$

and we now obtain the correct MFT exponents above d_c . [We omit here the specific heat and critical isotherm for which the same argument holds; Eqs. (11)-(12) deliver *all* mean-field exponents with y_t^* and y_h^* in place of the original scaling dimensions.] The finite-size behaviour is immediate by setting $b = L$ in Eqs.(14) and differentiating appropriately [12], e.g.

$$m_{T_c}(u, L^{-1}) \sim L^{-d/4}M(AL^{2-d/2}u^{1/2}), \quad (17)$$

$$\chi_{T_c}(u, L^{-1}) \sim L^{d/2}X(AL^{2-d/2}u^{1/2}). \quad (18)$$

If the finite-size correlation length were bounded by the system length [12], one could not write the combination $L^{y_t^*}t$, which enters the free energy, as a ratio L/ξ along the lines of Eq.(3). Within this framework, another length scale $\ell(t)$ was introduced, dubbed the thermodynamic length, with $\ell(t) \sim t^{-2/d}$, FSS being governed by the ratio $L/\ell(t)$ instead [13].

Contrary to previously widespread opinion [8, 12–17], the correlation sector also needs reexamination and the homogeneity assumption above d_c there takes the form [18]

$$\xi(t, u) = b^{\vartheta}\Xi \left(b^{d/2}\frac{t}{u^{1/2}} - Ab^{2-d/2}u^{1/2} \right), \quad (19)$$

$$g(t, u, \mathbf{x}) = b^{-d/2}G \left(b^{d/2}\frac{t}{u^{1/2}} - Ab^{2-d/2}u^{1/2}, b^{-1}\mathbf{x} \right), \quad (20)$$

where we omit the h -dependence for clarity. This leads to a new interpretation, dubbed QFSS in [19], above $d = d_c$ dimensions. [The “Q” refers to the introduction of a pseudocritical exponent ϑ which governs the FSS of the correlation length in Eq.(19).] The finite-size behaviour is transparent from Eqs.(19) and (20); fixing the scale factor $b = L$ we get

$$\xi_{T_c}(u, L^{-1}) \sim L^{\vartheta}\Xi(AL^{2-d/2}u^{1/2}), \quad (21)$$

$$g_{T_c}(u, \mathbf{x}, L^{-1}) \sim L^{-d/2}G(AL^{2-d/2}u^{1/2}). \quad (22)$$

Above the upper critical dimension, $\vartheta = d/d_c$ and the notion of thermodynamic length is abandoned in the QFSS picture [18–21]. Below d_c , $\vartheta = 1$ and ordinary FSS is recovered.

This picture is corroborated by analytical and numerical calculations for systems with periodic boundary conditions (PBC), both in the short-range Ising model (SRIM) above $d_c = 4$ and in long-range Ising model (LRIM) above $d_c = 2\sigma$ [18–21]. In the latter case, the general discussion has to be modified. The sum over interactions in Eq.(6) is extended to all pairs with decaying couplings $J_{\mathbf{x}-\mathbf{x}'} \sim J/|\mathbf{x} - \mathbf{x}'|^{d+\sigma}$. The MFT critical exponents of Eqs. (4) and (5) remain valid except that $\nu = 1/\sigma$ and $\eta = 2 - \sigma$, and the RG eigenvalues at the Gaussian FP take the form $y_t = \sigma$, $y_h = (d + \sigma)/2$, and $y_u = 2\sigma - d$ [22]. One recovers the SRIM values with $\sigma = 2$. The standard scaling laws (12) are satisfied above d_c while those of (11) are not, indicating again the dangerous irrelevancy of the quartic term in the action, which now contains an additional $|\mathbf{k}|^\sigma$ term. The modified (starred) RG dimensions are the same as before. The agreement between numerical results for PBC's and the scaling picture of Eqs. (17), (18), (21) and (22) is complete when simulations are performed at T_c , but also when they are performed at the pseudocritical point T_L (defined by the size-dependent temperature where a quantity such as the susceptibility exhibits a maximum).

When FBC's are imposed, there appears an intriguing feature. Simulation results are consistent with the above picture at the pseudocritical point T_L of the FBC system [19], but not at T_c where, instead, standard FSS with the Landau MFT-type exponents of Eq.(5) has been obtained *for the susceptibility* [23–27].

As recently shown by Wittman and Young [24] (see also [10, 11, 23]), the Fourier modes play a key role. The non-zero modes, which are not affected by DIV's, contribute to the FSS of the susceptibility with the Landau ratio $\gamma/\nu = 2$ for PBC's at both T_c and T_L and they argued for the same Landau behaviour of analogous modes for FBC's at T_L . We show below that standard FSS with Landau exponents is not correct; it is in conflict with the RG.

We follow Ref.[23] and perform a sine-expansion of the scalar field in Eq.(7) satisfying $\phi(\mathbf{x}) = 0$ at the free surfaces: $\phi(\mathbf{x}) = \sum_{\mathbf{k}} \phi_{\mathbf{k}} \prod_{\alpha=1}^d \sqrt{2/L} \sin k_{\alpha} x_{\alpha}$, where $k_{\alpha} = n_{\alpha} \pi / L$, $n_{\alpha} = 1, 2, \dots, L$. In $\mathbf{k}$ -space, the action takes a form slightly different to that for PBC's and one must distinguish modes for which all n_{α} -values are odd integers. These are analogous to the zero mode in the PBC case and we denote their set by Q . We denote the remaining modes by G . The action now reads [23]

$$S[\phi] = \frac{1}{2} \sum_{\mathbf{k}} \left(r_0 + c|\mathbf{k}|^2 \right) \phi_{\mathbf{k}}^2 - \left(\frac{8}{L} \right)^{\frac{d}{2}} h \sum_{\mathbf{k} \in Q} \phi_{\mathbf{k}} \prod_{j=1}^d \frac{1}{k_j} + \frac{u}{L^d} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4} \Delta_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4} \phi_{\mathbf{k}_1} \phi_{\mathbf{k}_2} \phi_{\mathbf{k}_3} \phi_{\mathbf{k}_4}, \quad (23)$$

where the Δ_i 's are momentum-conserving factors. The difference between the quadratic terms of Eqs.(13) and (23) is the source for the difference in scaling between the pseudocritical shifts in the PBC and FBC cases [23]. The quartic term in Eq.(23) is dangerous only for the modes $\mathbf{k} \in Q$ which couple to h . We henceforth refer to modes for which u is dangerous (in particular, the zero mode at T_c and T_L for PBC's and modes with all odd n_α at T_L for FBC's) as Q-modes and the remaining ones as Gaussian modes or G-modes.

We introduce the notation $m_{\mathbf{k}}$ to represent the contribution of a single mode $\mathbf{k}$ to the average magnetization. Thus $m_{\mathbf{k}} = \langle \phi_{\mathbf{k}} \rangle = \langle \int \phi(\mathbf{x}) \psi_{\mathbf{k}}(\mathbf{x}) d^d x \rangle$, where $\psi_{\mathbf{k}}(\mathbf{x})$ is the standing wave or the sine mode depending upon the BC's. The brackets indicate the thermal average with the Boltzmann weight corresponding to the action (13) or (23). The equilibrium magnetization is then $m = \langle \int d^d x \sum_{\mathbf{k}} \phi_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{x}) \rangle$. The Q-modes acquire non-vanishing expectation values and have projections onto the equilibrium magnetization m [23, 24]. The G-modes do not have such projections and were expected to exhibit standard FSS given by (3) with Landau exponents (5). This was supported by numerical evidence for the susceptibility Fourier modes $\chi_{\mathbf{k} \in Q}$ in [24].

Either we study physical quantities which are related to the Q-modes, in which case the DIV has to be properly taken into account, *or* we analyze properties associated with G-modes for which u is not dangerous. In the latter case the exponents are those predicted by the RG at the Gaussian FP; these are (11), (12), *and not Landau exponents* (4), (5). In the first case, on the other hand, the exponents are indeed MFT exponents (4), (5), but the correlation length has the FSS behavior involving ϑ and Eq.(3) has to be modified to QFSS which, e.g. for magnetization and susceptibility, reads as

$$m(t, L^{-1}) \sim m(t, 0) [L^\vartheta / \xi(t)]^{-\frac{\beta}{\nu}} \sim L^{-\frac{\vartheta\beta}{\nu}} \sim L^{-\frac{d}{4}}, \quad (24)$$

$$\chi(t, L^{-1}) \sim \chi(t, 0) [L^\vartheta / \xi(t)]^{\frac{\gamma}{\nu}} \sim L^{\frac{\vartheta\gamma}{\nu}} \sim L^{\frac{d}{2}}. \quad (25)$$

The Q-modes $m_{\mathbf{k} \in Q}$ and $\chi_{\mathbf{k} \in Q}$ themselves also obey QFSS. For G-modes this reduces to standard FSS:

$$m_{\mathbf{k} \in G}(t, L^{-1}) \sim m_{\mathbf{k} \in G}(t, 0) [L / \xi(t)]^{-(d-y_h)} \sim L^{-\frac{d-\sigma}{2}}, \quad (26)$$

$$\chi_{\mathbf{k} \in G}(t, L^{-1}) \sim \chi_{\mathbf{k} \in G}(t, 0) [L / \xi(t)]^{2y_h-d} \sim L^\sigma. \quad (27)$$

Eq.(27) agrees numerically with the result of Wittmann and Young [24] because the combination of exponents $2y_h - d$ equals σ and coincides with γ/ν (for the SRIM, $\sigma = 2$). However, there is no way to reconcile Eq.(26) with the power $-\beta/\nu = -\sigma/2$ ($= -1$ for the SRIM) for arbitrary d above $d_c = 2\sigma$. The long-standing puzzle associated with FBC's is due to the fact that if the

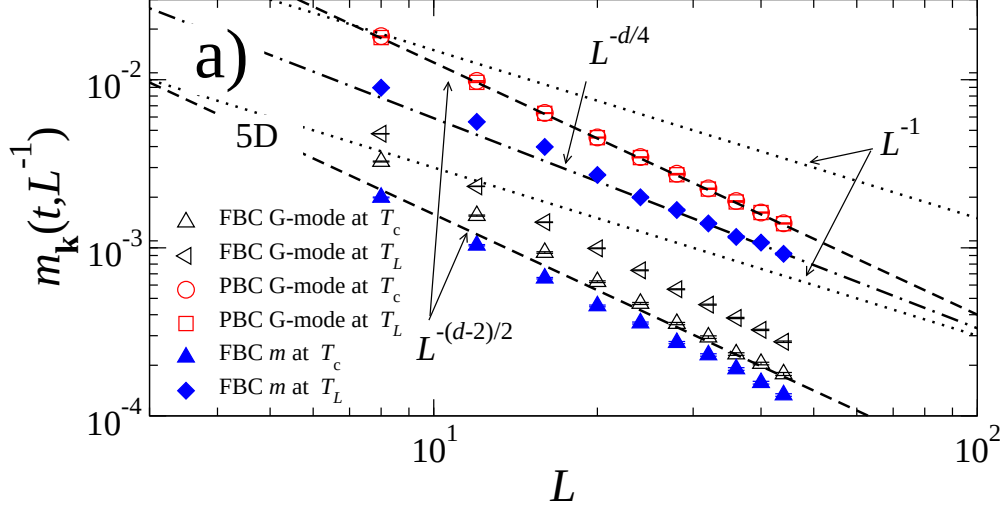


Figure 1: FSS for the 5D SRIM. The magnetisation for FBC's belongs to the DIV sector and scales as $m(T_L) \sim L^{-d/4}$ ($\blacklozenge$). At T_c the magnetization scales as $L^{-(d-2)/2}$ as predicted by Gaussian FSS ($\blacktriangle$). The remaining data are for the lowest critical and pseudocritical G-modes $m_{\mathbf{k}}(L^{-1})$, each of which belongs to the non-DIV sector. Here we see they also follow Gaussian FSS and not the Landau FSS prediction L^{-1} (which is indicated by the dotted lines).

Q-mode quantities follow Eqs. (24) and (25) at T_L , they fail at T_c and obey instead scaling given by Eqs. (26) and (27) like G-quantities.

In order to determine which of the forms (24) from QFSS, or (26) from the Gaussian FP, or $m \sim L^{-\beta/\nu} = L^{-\sigma/2}$ from Landau exponents in Eq.(3), correctly describes the scaling of the magnetization at T_c , we performed Monte Carlo simulations for the SRIM and the LRIM above d_c , along the lines described in [21]. The various sectors to be examined are summarised in Table I.

Since we are simulating with finite-size lattices, we examine the magnitudes of the G-mode contributions through $m_{\mathbf{k}}(L^{-1}) = \langle |s_{\mathbf{k}}| \rangle = \langle | \sum_{\mathbf{x}} s_{\mathbf{x}} \psi_{\mathbf{k}}(\mathbf{x}) | \rangle$, where $s_{\mathbf{x}}$ is an Ising spin at site $\mathbf{x} = \mathbf{n}\mathbf{a}$. The total magnetization is $m(L^{-1}) = \langle | \sum_{\mathbf{x}} s_{\mathbf{x}} | \rangle$. For the DIV sectors, scaling of the magnetization

Table I: The partitioning of Fourier modes into dangerous and non-dangerous sectors of the model. FSS in the Q (DIV) sector is given by Eqs.(24) and (25). For the G (non-DIV) sector, it predicts (26) and (27) while Landau FSS gives $m \sim L^{-\beta/\nu} = L^{-\sigma/2}$ and $\chi \sim L^{\gamma/\nu} = L^{\sigma}$ from (3).

	PBC		FBC	
	$k = \frac{2\pi}{L}(n_1, \dots, n_d)$		$k = \frac{\pi}{L+1}(n_1, \dots, n_d)$	
	$n_\alpha = 0 \forall \alpha$	$n_\alpha \neq 0$ for any α	All n_α odd	Any n_α even
T_L	Q-modes	G-modes	Q-modes	G-modes
T_c	Q-modes	G-modes	G-modes	G-modes

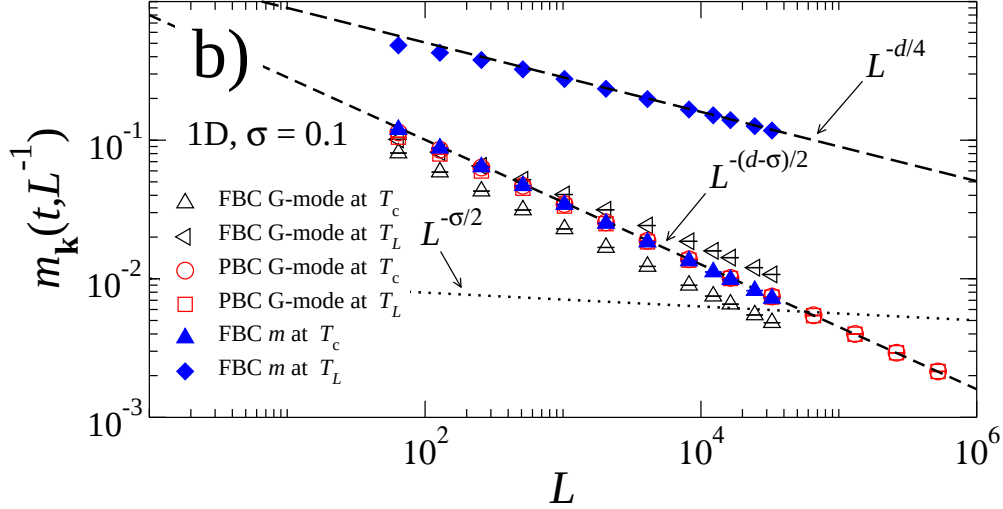


Figure 2: FSS for the 1D LRIM with $\sigma = 0.1$. As in Fig.1, the magnetisation for FBC's exhibits QFSS at T_L , scaling as $m(T_L) \sim L^{-d/4}$ ($\blacklozenge$) and Gaussian FSS at T_c scaling as $L^{-(d-\sigma)/2}$ ($\blacktriangle$). The lowest critical and pseudocritical G-modes all also follow Gaussian FSS and not the Landau FSS prediction $L^{-\sigma/2}$ (which is indicated by the dotted line).

follows $m(L^{-1}) \sim L^{-d/4}$ from Eq.(24). For PBC's at T_c , this is already well established, having also been verified numerically in [28]. We find the same behaviour for PBC's at T_L . Results for FBC's at T_L support the same scaling there for both the SRIM and the LRIM. For the non-DIV sectors, standard FSS with Landau exponents predicts $m(L^{-1}) \sim L^{-\sigma/2}$ while we predict Gaussian scaling $m(L^{-1}) \sim L^{-(d-\sigma)/2}$ after Eq.(26). For the 5D SRIM, then, a plot on a double logarithmic scale should have slope -1 according to “Landau FSS” or $-3/2$ according to Eq.(26). Our results in Fig.1 are clearly compatible with the latter and rule out the former. For the LRIM above d_c the outcome is even more stark; “Landau FSS” predicts a slope of $-\sigma/2 = -0.05$ independent of d and Eq.(26) predicts $-(d-\sigma)/2 = -0.45$, for $d = 1$, the latter being clearly favoured by the data in Fig. 2.

In the literature, it has been stated that “due to the lack of a better way of treating the zero-momentum modes” it is usual to “neglect them completely” [29]. Standard phenomenological FSS associated with the excited modes was then expected to deliver “Landau FSS”. The results established here indicate that this approach is not correct. Also in the literature, the critical exponents (11) and (12) are presented as non-physical; they were hitherto merely a step on the way to reconciling RG theory with Landau mean-field exponents above d_c . Here we have shown that they are, in fact, physically manifest in the magnitudes of the G-modes. This is not a feature of finite size only. In the thermodynamic limit, G-modes would, for example acquire the temperature

behaviour $m_{\mathbf{k} \in G}(t) \sim |t|^{d/2\sigma-1/2}$. Moreover, mean-field theory fails to fully describe either G- or Q-modes above the upper critical dimension. Instead this careful approach to RG, taking QFSS into account, delivers a consistent description for all Fourier modes.

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