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2010 J. Phys. A: Math. Theor. 43 125002

(http://iopscience.iop.org/1751-8121/43/12/125002)

IOP Publishing — Journal of Physics A: Mathematical and Theoretical

J. Phys. A: Math. Theor. **43** (2010) 125002 (9pp) doi:10.1088/1751-8113/43/12/125002

Local scale invariance for wetting and confined interfaces

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Received 22 January 2010
Published 4 March 2010
Online at stacks.iop.org/JPhysA/43/125002

Abstract

When a fluid or Ising-like magnet is confined between two parallel walls that are each completely wet by different bulk phases, the interface separating the phases is subject to large-scale fluctuations determined by the slit width. It was noted some time ago that, in two dimensions, the scaling expression for the probability distribution function describing the interfacial height across the slit shows remarkable similarities with predictions of conformal invariance. However, this local scale invariance appears to contradict the strongly anisotropic nature of (1 + 1)-dimensional interfacial fluctuations along and perpendicular to the interface, characterized by the wandering exponent. In this paper, we show that similarity with conformal invariance is not coincidental and can be understood explicitly as the projection of a local scale invariance for a wandering line in 2 + 1 dimensions.

PACS numbers: 68.08.Bc, 05.70.Fh, 05.70.Np

1. Introduction

The behaviour of fluid interfaces in confined geometries has received enormous attention over the last 20 years. A well-studied example of this is fluid confinement in a parallel-plate (capillary-slit) geometry in which each wall preferentially adsorbs a different bulk phase [1–5]. In this case, the fluid phase behaviour is very different to that occurring for confinement between identical walls, and is determined by length-scales related to wetting transitions. This geometry is very convenient for simulation studies [6, 7] and other numerical approaches such as the density-matrix renormalization group [8], and has revealed a great deal about the scaling behaviour arising from interfacial fluctuation effects and also wetting-induced delocalization transitions. One peculiar feature of such interfacial confinement in two dimensions (i.e. a one-dimensional interface) that has not been understood, concerns the apparent conformal invariance of an important observable—the probability distribution function (PDF) for the interface position [9]. To be more specific, analytic expressions for the PDF, as determined

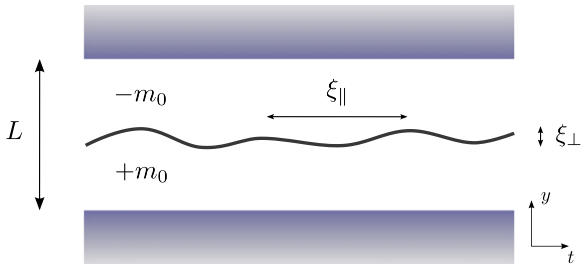

Figure 1. Schematic illustration of a confined interface in a two-dimensional Ising strip with opposing surface spins, below the bulk critical temperature. The interface separating up-spin and down-spin phases is subject to large-scale and strongly anisotropic fluctuations characterized by the correlation lengths $\xi_\parallel$ and $\xi_\perp$ along and across the strip. In coarse-grained effective Hamiltonian descriptions, the interfacial configuration is described by the collective coordinate $y(t)$.

exactly in model calculations, are precisely of the form that would be expected if conformal invariance were obeyed. However, the presence of such an underlying isotropic local scale invariance is highly unexpected since it is well appreciated that fluctuating interfaces exhibit strongly anisotropic scaling in directions parallel and perpendicular to the interface [10, 11]. Indeed, this anisotropic scaling forms the basis for all renormalization group theories of wetting [11, 12]. In this paper, we present a simple argument (based on a transfer-matrix formulation) which shows how the conformal invariance for the interfacial height PDF in (1 + 1)-dimensional systems arises from local scale invariance properties of random walks in 2 + 1 dimensions and complements, rather than contradicts, the basic anisotropic scaling of fluctuating interfaces. We begin our paper by recalling some background theory, concerning the finite-size scaling behaviour of confined interfaces (below the bulk critical point), and the strong similarities these results bear with predictions of conformal invariance for the finite-size scaling of the magnetization profile exactly at criticality.

2. Background theory

2.1. Finite-size scaling of an interface between two walls

Consider a two-dimensional square lattice Ising model of infinite length and finite width L (measured in units of the lattice spacing). We suppose that the bulk magnetic field is zero but that the surface spins are fixed to +1 and −1 along the lower and upper edges (walls) of the strip, respectively (see figure 1). Below the bulk critical temperature $T < T_c$, these asymmetric boundary conditions induce the formation of a one-dimensional interface separating up-spins (below it) and down-spins (above it), that runs along the length of the strip. The interface is unbound from both the lower and upper walls since these are completely wet by the up-spin and down-spin bulk phases, respectively. Provided the width L is much bigger than the bulk correlation length, the fluctuations of this interface are extremely large, and lead to scaling behaviour in the magnetization profile, energy density and their correlations. This scaling is strongly anisotropic and is characterized by length-scales $\xi_\perp \propto L$ and $\xi_\parallel \propto L^2$, perpendicular and parallel to the interface, respectively [4]. The relation between these length-scales, $\xi_\perp \approx \xi_\parallel^\zeta$, identifies the thermal value of the wandering exponent $\zeta = 1/2$, for one-dimensional interfaces [13], which plays a crucial role in fluctuation theories of wetting. Consider, for example, the equilibrium value of the local magnetization at a perpendicular distance y from the lower wall, again measured in units of the lattice spacing. For fixed

$T < T_c$, and in the limits $y \to \infty$ and $L \to \infty$ with y/L arbitrary, we anticipate the scaling law $m(y) = m_0 M(y/L)$ where m_0 is the spontaneous magnetization and $M(Y)$ is a scaling function. Exact calculations determine the precise expression of this scaling function as [14]

$$\frac{m(y)}{m_0} = 1 - \frac{2y}{L} + \frac{1}{\pi}\sin\left(\frac{2\pi y}{L}\right). \tag{1}$$

On the other hand, the two-point spin–spin correlation function between spins at coordinates y_1 and y_2, separated by a distance t_{12} along the strip, scales as $G(y_1, y_2; t_{12}) = m_0^2 M_2(y_1/L, y_2/L; t_{12}/L^2)$, reflecting the anisotropy of interfacial fluctuations and the dependence on the dimensionless variable $t_{12}/\xi_\parallel$. The reason we have chosen the variable t, rather than x, to denote the distance along the strip will be clear later. Similar scaling is present in the properties of the energy-density operator (the product of nearest-neighbour spin variables at positions y and $y+1$) and its correlations. For example, the one-point function contains a singular contribution that scales as [14]

$$\frac{\epsilon(y)}{\sigma} = \frac{2}{L}\sin^2\left(\frac{\pi y}{L}\right), \tag{2}$$

where σ is the surface tension of the up-spin/down-spin interface.

The above scaling expressions, which emerge from very involved transfer-matrix analysis of the microscopic Ising model, were first predicted using a much simpler continuum effective interfacial Hamiltonian [4, 9]. Let $y(t)$ denote the local height of the interface at position t along the strip. The energy cost of an interfacial configuration is written, phenomenologically, as

$$H[y] = \int \mathrm{d}t \left\{ \frac{\Sigma}{2}\dot{y}^2 + W(y) \right\}, \tag{3}$$

where Σ is the interface stiffness coefficient, $\dot{y} = \mathrm{d}y/\mathrm{d}t$ and $W(y)$ is the binding potential which models the confinement and the interaction with the walls. Obviously, this interfacial description is only valid below the bulk critical temperature and for slit widths much larger than the bulk-correlation length. This is sufficient to capture the precise scaling behaviour induced by the wandering of the domain wall. The transfer-matrix analysis of the interfacial model is straightforward and, in the limit of infinite (momentum) cut-off, is equivalent to a path integral [15, 16]. Thus, the spectrum is determined from the solution of the Schrödinger-like ordinary differential equation

$$-\frac{1}{2\Sigma\beta^2}\frac{\mathrm{d}^2\psi_n(y)}{\mathrm{d}y^2} + W(y)\psi_n(y) = E_n\psi_n(y), \tag{4}$$

where $\beta = 1/k_B T$. In particular, for the present problem of an infinitely long strip, the probability of finding the interface at distance y above the lower wall is simply $P(y) = |\psi_0(y)|^2$. This directly determines the energy density and magnetization profiles using $\epsilon(y) = \sigma P(y)$ and $m(y) = m_0\big(1 - 2\int_0^y P(\tau)\,\mathrm{d}\tau\big)$, respectively. In addition, the associated ground-state energy E_0 determines the singular contribution to the excess free energy per unit length. For Ising-like systems with purely short-ranged forces, one may approximate the binding potential as an infinite square well, $W(y) = 0$ for $0 < y < L$ and $W(y) = \infty$ otherwise, which simply models two hard-wall repulsions. The ground-state wavefunction $\psi_0(y) \propto \sin(\pi y/L)$ then leads to

$$P(y) = \frac{2}{L}\sin^2\left(\frac{\pi y}{L}\right) \tag{5}$$

and, hence, to the scaling expressions for $\epsilon(y)$ and $m(y)$ quoted above. For our purposes, it is relevant that the PDF has a characteristic power-law or short-distance expansion

$$P(y) \propto y^2; \qquad y/L \ll 1 \tag{6}$$

as the scaling variable $y/L \to 0$. This power law has a more general significance and is also obtained when one considers the complete wetting transition, occurring at a single wall, from off bulk coexistence [17]. To see this, consider a semi-infinite Ising model, with surface spins fixed to +1, but now with a negative bulk magnetic field, h, implying that the spins far from the wall have a net negative magnetization. As the strength of the magnetic field is reduced, the thickness of the adsorbed layer of up-spins near the wall diverges [11, 18, 19]. One may model this using the interfacial model (3) with the binding potential $W(y) = 2m_0|h|y$ (for $y > 0$), from which it follows that the mean wetting layer thickness grows as $\langle y\rangle \approx |h|^{-1/3}$ [15, 20]. The PDF for the interfacial height also shows scaling in this limit, and can be written as $P(y) \approx \langle y\rangle^{-1}\Phi(y/\langle y\rangle)$, where $\Phi(Y)$ is a universal scaling function (the square of an Airy function). For fixed y (far from the wall) and $h \to 0$, corresponding to the scaling variable $Y \to 0$, the scaling function has the short-distance expansion, $\Phi(Y) \approx Y^2$, and is the same as the power law shown in (6). More generally still, for systems with short-ranged forces, the divergence of the film thickness and the power law of the short-distance expansion of the PDF, at fluctuation-dominated complete wetting transitions, are determined by the value of the wandering exponent [10, 11, 17]: $\langle y\rangle \approx |h|^{-\zeta/(2-\zeta)}$ and $P(y) \propto y^{2(1/\zeta-1)}$. These recover the results quoted above on setting $\zeta = 1/2$, corresponding to the thermal wandering of a one-dimensional interface.

Returning to the strip geometry, we note that (according to the interfacial description) the results (1) and (2) remain valid and represent universal scaling behaviour, provided that the tails of the binding potential decay faster than the inverse square of the distance from each wall. This corresponds to the fluctuation-dominated regime of 2D complete wetting transitions. For more slowly decaying potentials, interfacial fluctuation effects are less strong, with $\xi_\perp \ll L$ for large strips widths, and do not lead to simple universal scaling behaviour. It is instructive to consider the marginal boundary between these fluctuation-dominated and mean-field-like regimes in more detail. Let us consider the semi-infinite geometry first and consider the complete wetting transition with a marginal binding potential $W(y) = 2m_0|h|y + By^{-2}$. For simplicity, we will take $B > 0$ to avoid the complication of a wetting transition, corresponding to binding the interface to the wall when B is sufficiently negative [21]. The presence of the marginal inverse-square tail does not change the critical exponent for the growth of the wetting layer, $\langle y\rangle \approx |h|^{-1/3}$, although the amplitude is altered. The transition is still characterized by large interfacial fluctuations and the PDF for the interfacial height still shows scaling such that $P(y) \approx \langle y\rangle^{-1}\Phi_B(y/\langle y\rangle)$. However, the short-distance expansion of the scaling function is strongly influenced by the marginal interaction, and for fixed y and $h \to 0$, shows a power law

$$P(y) \propto y^{2\phi}. \tag{7}$$

where $\phi = (1 + \sqrt{1 + 8\beta^2\Sigma B})/2$. Now consider the analogous finite-size scaling behaviour for an interface in a strip geometry with marginal forces. We require that, in the limit of large L, the binding potential decays as an inverse square of the distance from each wall. There are, of course, many potentials that decay in this fashion, for example the simple linear combination $W(y) \approx y^{-2} + (L - y)^{-2}$. Instead, however, we consider interfacial confinement described by the marginal binding potential

$$W(y) = \frac{B\pi^2}{L^2}\sin^{-2}\left(\frac{\pi y}{L}\right) \tag{8}$$

with $W(y) = \infty$ for $y < 0$ and $y > L$. The reason for this choice will become clearer later. Again, for simplicity, we assume $B > 0$ so that the walls are completely wet by the appropriate bulk phase. Note that, in the limit $L \to \infty$, the binding potential behaves as a pure inverse-square power law at finite distances from each wall. The ground-state wavefunction, for the marginal potential (8), is simply $\psi_0 \propto \sin^\phi(\pi y/L)$ leading to

$$P(y) \propto \sin^{2\phi}\left(\frac{\pi y}{L}\right), \tag{9}$$

while the corresponding eigenvalue is

$$E_0 = \frac{\pi^2\phi^2}{2\Sigma\beta^2 L^2}. \tag{10}$$

Setting $B = 0$, recovers the universal behaviour indicative of short-ranged forces, discussed above.

2.2. Similarities with conformal invariance

The above results bare a strong similarity to universal finite-size scaling behaviour in 2D systems occurring exactly at the bulk critical point. Consider a semi-infinite Ising model whose surface spins are fixed to +1 and again denote the coordinate perpendicular to the edge (wall) by y. Let us now denote the coordinate parallel to the edge by the more traditional variable x. Exactly at the bulk critical temperature $T = T_c$ and in zero bulk field, scaling theory implies that, at large distances, the magnetization profile necessarily decays as a universal power law [22–24]

$$m(y) \approx Ay^{-\beta/\nu}, \tag{11}$$

where $\beta = 1/8$ and $\nu = 1$ are the well-known 2D critical exponents for the spontaneous magnetization and bulk correlation length, respectively, and A is an unimportant metric factor. Now, consider the related finite-size scaling of the magnetization profile occurring at the bulk critical point in an infinitely long Ising strip of width L, but with symmetric boundary conditions that fix the spins to +1 at upper and lower edges. Following the scaling theory of Fisher and de Gennes [23], in the limit $y \to \infty$ and $L \to \infty$ with y/L fixed, the magnetization profile behaves as $m(y) = AL^{-\beta/\nu}M_c(y/L)$, where $M_c(Y)$ is a universal scaling function. Burkhardt and Eisenreigler [25] pointed out that the scaling function can be determined using a simple argument based on conformal invariance. The power law (11) implies that magnetization transforms as $m(y/b) = b^{\beta/\nu}m(y)$ under a global spacial rescaling by a factor b. The assumption of a local conformal invariance generalizes this co-variance law to

$$m(u, v) = |w'(z)|^{-\beta/\nu}m(y), \tag{12}$$

where $w(z) = u + \mathrm{i}v$ is an analytic function that maps the original plane $z = x + \mathrm{i}y$ to new coordinates (u, v). Using $w(z) = (L/\pi)\ln z$ to map the semi-infinite plane to the infinite strip $(0 < v < L, -\infty < u < \infty)$, they predicted

$$m(v) \approx AL^{-\beta/\nu}\sin^{-\beta/\nu}\left(\frac{\pi v}{L}\right), \tag{13}$$

which has been tested and confirmed in subsequent studies [26].

There is, therefore, a remarkable similarity between the expression for the magnetization profile (13), pertinent to the symmetric Ising strip at bulk criticality, with the result (5) for the interfacial height PDF (and its generalization (9), for marginal forces), in the asymmetric Ising strip, for $T < T_c$. It is tempting to conjecture [9] that some aspect of conformal invariance applies to interfaces, and that one may similarly use the logarithmic map $w(z) = (L/\pi)\ln z$ to transform the short-distance expansion (7) into (9). In other words, a similar covariance law to (12) also holds for the PDF for wetting transitions but with the appropriate short-distance expansion exponent 2ϕ replacing $-\beta/\nu$. This is all the more appealing because the marginal binding potential (8) is also obtained by logarithmically mapping the pure power-law $W(y) = By^{-2}$ to the strip geometry.

However, there is a serious problem with this conjecture as it appears to contradict the anisotropic scaling associated with interfacial fluctuations. Recall that conformal invariance implies that local scale dilations are isotropic. In the transformation (12), both x and y coordinates rescale with the same local dilation factor. As stressed above, scaling and associated scale invariance for interfaces is strongly anisotropic. For example, the free part (gradient term) in the interfacial Hamiltonian (3) is invariant under a spacial rescaling $y \to y/b_\perp$ and $t \to t/b_\parallel$, where $b_\perp = \sqrt{b_\parallel}$ (as required by the value of the wandering exponent $\zeta = 1/2$). Any local version of this scale invariance cannot be conformal. In addition, if some aspect of conformal invariance did apply to interfaces, one would like to understand how it arises explicitly in the transfer-matrix formulation.

3. Local scale invariance of a fluctuating line in 2+1 dimensions

The similarity between the results for finite-size scaling in critical Ising strips and for confined interfaces is, in fact, not coincidental. To see how it arises, we note that the behaviour of a confined interface in 1 + 1 dimensions shares a great deal in common with the properties of a fluctuating line in 2+1 dimensions. In both cases, the object that fluctuates is one dimensional and analogous to the motion of a random-walk. The apparent conformal invariance for the interfacial problem is a projection of an explicit conformal invariance for this higher dimensional problem describing the wandering line. However, the geometrical meaning of this mapping is not the same as in the standard application of conformal invariance in the critical Ising strip. In particular, it does not refer to the direction parallel to the interface (which we denoted as t) and hence does not invoke the anisotropic scaling factors $b_\perp$ and $b_\parallel$. Rather it refers to the two-dimensional plane perpendicular to t.

To make these ideas explicit, consider the statistical mechanics of a one-dimensional directed line in a 3D space (see figure 2). The line no longer represents a domain wall but can be thought of representing a wandering directed polymer strand. The coordinate parallel to the principle direction of the line is written as t while, in the plane perpendicular to this, the coordinates $(x(t), y(t))$ describe its location parametrically. Neglecting overhangs and assuming that fluctuations from a straight-line configuration are relatively small, we suppose that the energy cost of a configuration is given by the effective Hamiltonian

$$H[x, y] = \int \mathrm{d}t \left\{ \frac{\Sigma}{2}(\dot{x}^2 + \dot{y}^2) + W(x, y) \right\}. \tag{14}$$

Here, Σ is a line-tension-like quantity as opposed to a surface tension, and W is a binding potential which now depends on two coordinates. Mathematically, this is just the (2 + 1)-dimensional version of the (1 + 1)-dimensional interfacial Hamiltonian described earlier (3). The motion of this line is similar to that of the interface and is characterized by the same wandering exponent. That is the free Hamiltonian is invariant under $(x, y) \to (x/b_\perp, y/b_\perp)$ and $t \to t/b_\parallel$ with $b_\perp = \sqrt{b_\parallel}$. In the limit of infinite cut-off, the partition function sum is again equivalent to a path integral and the transfer-matrix spectrum is found from solution of the two-dimensional Schrödinger equation $\hat{H}\psi_n(x, y) = E_n\psi_n(x, y)$ where

$$\hat{H} = -\frac{1}{2\Sigma\beta^2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + W(x, y). \tag{15}$$

As before, for an infinitely long system and any fixed value of t, the probability of finding the line at a given location is determined by the ground state $P_2(x, y) = |\psi_0(x, y)|^2$, where

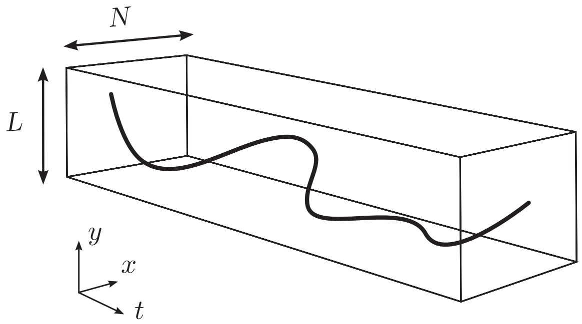

Figure 2. Schematic illustration of a wandering line in an infinitely long (2 + 1)-dimensional confined geometry with periodic boundary conditions in the x direction. The probability of finding the line at a given height is the same as the corresponding PDF for the confined interface shown in figure 1.

the subscript refers to the two dimensions of the (x, y) plane. Integrating this w.r.t x, $P_2(y) = \int \mathrm{d}x |\psi_0(x, y)|^2$, generates the probability of finding the line at any height y.

Consider the behaviour of the line interacting with a bounding plane which restricts its motion to the semi-volume $y > 0$. Suppose, for example, the potential is given by $W(x, y) = 2m_0 |h| + By^{-2}$ so that the line is free to wander parallel to the plane, but is bound in the perpendicular direction to it. As $h \to 0$, the line unbinds from the plane, analogous to the interfacial unbinding (complete wetting) transition in 1 + 1 dimensions described earlier. In this limit, the eigenvector equation for the ground state reads

$$-\frac{1}{2\Sigma\beta^2}\frac{\partial^2\psi_0(x, y)}{\partial y^2} + W(x, y)\psi_0(x, y) = 0 \tag{16}$$

where we have used the fact that the ground state is independent of x. The solution to this equation, neglecting normalization constants, is $\psi_0(x, y) \propto y^\phi$ where $\phi = (1 + \sqrt{1 + 8\beta^2\Sigma B})/2$ is the same short-distance expansion exponent that appeared earlier for the marginal interfacial problem. Next, consider a logarithmic coordinate mapping of the (x, y) plane: $z = x + \mathrm{i}y \to w(z) = u + \mathrm{i}v$ with $w = L/\pi \ln z$. These coordinates are perpendicular to the direction of the line, and are subject to the same isotropic local dilation. If we also map the wave-function according to

$$\psi_0(u, v) = |w'(z)|^\phi \psi_0(x, y), \tag{17}$$

then the differential equation (16) transforms to

$$-\frac{1}{2\Sigma\beta^2}\frac{\partial^2\psi_0(u, v)}{\partial v^2} + \overline{W}(u, v)\psi_0(u, v) = \frac{\pi^2\phi^2}{2\Sigma\beta^2}\psi_0(u, v), \tag{18}$$

where $\overline{W}(u, v) = (B\pi^2/L^2)\sin^{-2}(\pi v/L)$. This is the correct ground-state eigenvector equation for a line confined between two planes, separated by a distance L. Note there is no $\partial^2\psi/\partial u^2$ term due to translational invariance. The transformation (17), generates not only the appropriate bound-state wavefunction $\psi_0(u, v) \propto \sin^\phi(\pi v/L)$ but also identifies the ground-state energy for the transformed potential $\overline{W}(u, v)$. This is an explicit demonstration of local scale invariance for the wandering line in 2 + 1 dimensions within the transfer-matrix formalism. Clearly, the apparent conformal invariance for the confined interface is a projection of this, owing to the translational invariance in the u direction. Indeed, precisely the same ground-state wavefunction (up to a trivial normalization factor) and energy (10) describe the motion of the line, if one supposes that the system is finite in the u-direction with periodic boundary conditions in the planes $u = 0$ and $u = N$ (say). The normalized PDF for the height $P_2(y) \propto \sin^{2\phi}(\pi y/L)$ is independent of N. The small-N limit of this has the same interpretation as the interfacial problem.

4. Discussion

The above demonstration clarifies the status of the original conjecture concerning the possible application of conformal invariance to confined interfaces. The similarity between (9) and (13) is not coincidental, and the result (9) can indeed be obtained by conformally mapping a power-law short-distance expansion. However, the original interpretation and reasoning behind this [9] were not correct, and are different to the application of conformal invariance to the critical Ising strip (12). As we have shown, the conformal invariance actually applies to the motion of a wandering line in the plane perpendicular to its principle direction. This is the reason why it does not contradict the required anisotropy of scaling in the parallel and perpendicular directions.

On the negative side, these remarks seem to suggest that this type of local scale invariance has only limited applications for confined interfaces. Being a projection of the conformal invariance for the line in 2 + 1 dimensions, the mapping must preserve translational invariance in the hidden u dimension, which is extremely restrictive. Nevertheless, there are possible extensions of this approach which warrant further investigation. The first is straightforward. In the original discussion of possible local scale invariance for confined interfaces, it was noted that other properties, related to higher states of the transfer-matrix spectrum, appear to map conformally. It appears very likely to us that this has a similar explanation and involves the projection of invariant properties of the spectrum describing the wandering line. One might also like to investigate if the conformal invariance applies in systems where the wandering exponent is different to its thermal value. It might appear that the above argument, based on local scale invariance of the fluctuating line, is independent of the value of the wandering exponent since it does not invoke the anisotropic scaling of the (x, y) plane and t direction. However, this is not the case since, as remarked earlier, the value of the exponent ϕ appearing in the short-distance expansion of the PDF near one wall depends on ζ. There are a number of ways of altering the value of the wandering exponent, for instance, by modelling the presence of random-bond-like disorder [11]. Alternatively, one may use substrate geometry to influence the interfacial fluctuations. For example, the unbinding of an interface in a three-dimensional wedge can be described by a one-dimensional Hamiltonian in which the effective tension depends on the height from the wedge bottom [27]. The transfer-matrix analysis of this is now equivalent to quantum mechanics with a position-dependent mass, and alters the value of the wandering exponent to $\zeta = 1/3$ [28, 29]. One might be able to use a generalization of the above local scale invariance argument to this system in order to predict finite-size effects in 'double-wedge' geometries, similar to those employed in simulation studies. Finally, one would like to understand what aspects of local scale invariance apply to two-dimensional membranes. It is already known, from scaling and renormalization group arguments, that the fluctuations of two-dimensional membranes and one-dimensional interfaces are related precisely to each other [30]. The demonstration of conformal invariance for interfaces provided here leaves open the possibility that similar aspects apply to membranes.

Acknowledgments

CR acknowledges support from grants MOSAICO (Ministerio de Educacion y Ciencia) and grant 2009/00156/001 (Comunidad de Madrid/UC3M).

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