From surface to random criticality in layered planar Ising models.

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Abstract

A general case of a spatially nonuniform planar layered Ising model, or an equivalent quantum Ising chain, is analysed with an exact functional real space renormalization group. Various surface, finite size, quasiperiodic and random layer (McCoy-Wu) universality classes are obtained and discussed within a single theoretical framework leading to new insights into the nature of random criticality.

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While equilibrium critical phenomena in spatially uniform systems are gradually becoming a standard textbook chapter, much less is known about the way the critical state of matter is altered by the presence of spatial inhomogeneities of a general form. Models with uniformly distributed point disorder, on one hand, and with a planar surface, on the other, have attracted considerable attention and considerable progress in understanding of both has been achieved. However, the developments along these two directions have been largely independent, leaving a whole range of inhomogeneities largely unexplored. Important examples falling into this range are, to name just two, disordered quantum systems [1], in the path integral representation of which the disorder is fully correlated in the time direction, and fluids in porous media [2], in which case disorder enters in the form of random surfaces.

Here I am attempting to bridge this gap by presenting a new analysis of the class of layered planar Ising (LPI) models. A layered Ising model [3] is defined as having its bond strengths depending in an otherwise arbitrary way on just one of the \( d \) spatial coordinates, \( z \); in each layer perpendicular to that coordinate the bonds are of the same strength. These models may be viewed as a natural step in generalization of models with one planar surface towards the complexity of real systems. In particular, any LPI model is equivalent to an \( s = 1/2 \)-quantum Ising chain in transverse field which, depending on the way the transfer matrix is applied, can be made inhomogeneous either in space or in time. Besides, the rapidly developing technology of artificially grown multilayers provides natural experimental realizations of the layered geometry. Starting from the pioneering work of McCoy and Wu [4], a number of LPI models, both with surfaces and randomness [3], have been solved exactly. Subsequent scaling analysis of the exact solutions for surface and film geometries has played a crucial role in formulating surface [5] and finite size scaling [6]. More recently important progress has been made towards understanding of the random layer model [7], so the whole class seems to be a good testing ground for unifying ideas.

This work builds upon the microcanonical density functional method, proposed recently by M. E. Fisher and the author. Exact Euler-Lagrange equations obtained for the LPI class in [3] are used to construct a functional renormalization group (RG) flow in the space of
energy density profiles. Solving for the fixed points of this flow generates a list of universality classes found in LPI models. Common features of the flow in the vicinity of the fixed points describing the free film and random criticalities leads to interpretation of the latter as a hierarchy of thin-thick film crossovers with a significant element of quasi-one-dimensional behavior. This qualitative insight allows then for quantitative predictions to be made regarding critical behavior in quasiperiodic and long-range-correlated random sequences.

The Euler-Lagrange equations found in [3],

$$q \frac{\varepsilon_q(z) - (2q)^{-2}\dot{\varepsilon}_q(z)}{[1 - \varepsilon_q^2(z) + (2q)^{-2}\dot{\varepsilon}_q(z)^2]^{1/2}} = t(z),$$

describe the response of the energy density components $\varepsilon_q(z)$ to the scaled temperature field $t(z)$, which characterizes deviation from criticality of the local bond strengths in a given LPI model. Here $q$ is the wave number in the direction parallel to the layers, $\varepsilon_q(z)$ is the contribution to the total energy density from the excitations belonging to the $q$-sector of the equivalent fermion problem $[3, 8]$: $\dot{\varepsilon}_q(z) \equiv d\varepsilon_q/dz$, etc. An inverse lattice constant has been absorbed into the definition of $t$, giving it the proper scaling dimension of inverse length; the normalization of $[3, 10]$ makes the absolute value $|t| = |\xi^{-1}(z)|$, where $\xi(z)$ is the correlation length of a uniform model with the same bond strengths as the given $z$-layer (recall that $\xi \propto |t|^{-1}$ in a uniform planar Ising model). In this formalism the vertical bonds (connecting subsequent layers) have to be ferromagnetic, but the horizontal bonds can take either sign thus allowing for restricted forms of frustration (cf. [3]). Eqs. 1 are exact in the scaling limit $t(z) \ll \Lambda$, with the cutoff $\Lambda$ being of the order of the inverse lattice spacing. They have to be solved for every $q$ between 0 and $\Lambda$; after that the energy density, free energy, etc., are obtained by integration over $q$ of simple functions of $\varepsilon_q(z)$ and $\dot{\varepsilon}_q(z)$. This program has been explicitly carried out for simple surface $[3]$ and superlattice $[10]$ geometries, as represented by step-function and periodic $t(z)$, respectively.

In the latter case, apart from the information obtained from the explicit expressions for the free energy and total energy density profiles, it turned out to be instructive to study evolution of the partial energy density profiles $\varepsilon_q(z)$ in the long wave length limit $q \to 0$;
that evolution resembled many features of a functional renormalization group. Indeed, taking a partial derivative of the left hand side of (1) with respect to the logarithmic length scale along the layers, \( l = \ln(\Lambda/q) \), one obtains a partial differential equation depending only on \( \varepsilon_q \), its first two spatial derivatives, and, generally, on \( q = \Lambda e^{-l} \) as well. In this approach, the field \( t \) can be viewed as fixing the initial data at large \( q = \Lambda \), where \( \varepsilon(z;l=0) \approx t(z)/\Lambda \). The evolution of profiles as the logarithmic length scale \( l \) increases follows then its own dynamics, independent of the source \( t \), which, according to (1), becomes an integral of motion for this flow. The simplest illustration is provided by the uniform limit \( t = \text{const}, \partial\varepsilon/\partial z = 0 \). Differentiating both sides of (1) with respect to \( l \) gives then

\[
\partial\varepsilon/\partial l = \varepsilon(1 - \varepsilon^2).
\] (2)

As anticipated, Eq. 2 has three fixed points: \( \varepsilon = 0, \pm 1 \). In the scaling regime, \( t \ll \Lambda \), the flow always starts in the vicinity of the ultraviolet-stable critical fixed point \( \varepsilon = 0 \) and then takes the system either to the high-temperature, \( \varepsilon = 1 \), or to the low-temperature, \( \varepsilon = -1 \), fixed point, depending on whether the initial value \( \varepsilon(l = 0) = t/\Lambda \) is positive or negative, correspondingly. The eigenvalue \( \lambda_t = 1 \) governing the flow out of the critical fixed point, \( \partial\varepsilon/\partial l \approx \lambda_t \varepsilon \), gives the correct value of the correlation length exponent \( \nu = 1/\lambda_t = 1 \).

The general case of position dependent \( t \) requires supplementing flow in \( q \) with rescaling \( \varepsilon \to \varepsilon \exp(-\omega_z l), \ z \to z \exp(-\omega_z l) \), where the scaling dimensions \( \omega_z, \ \omega_z \) are tuned to achieve nontrivial fixed point structure and make the RG equations \( l \)-independent. In practice, it is easier to work with the integral of motion (1): each RG fixed point profile

\[
\varepsilon_q(z) = q^{\omega_z} \mathcal{E}(q^{\omega_z} z)
\] (3)

has to satisfy (1) with the same \( t(z) \) for every small \( q \). A straightforward analysis yields several fixed points.

First, at \( \omega_z = 0, \omega_z = 1 \) one finds the profile

\[
\mathcal{E}(y) = -\int^y dz \sinh(g(z)),
\] (4)
describing relaxation towards the uniform critical fixed point profile $\varepsilon \equiv 0$. The \textit{thermal potential}

$$g(z) = 2 \int z t(z_1) dz_1,$$  \hspace{1cm} (5)

will play a crucial role below. The condition of criticality in a layered Ising model discussed in [3] can be made more precise now: for (8) to make sense there has to exist a choice of integration constant in (5) such that the integral in (4) is bounded for all $y$ (note that $\varepsilon$ cannot exceed unity). This rather stringent constraint is satisfied in the critical state of a periodic [10] and, as one will see below, simple quasiperiodic LPI models, but not at the ferromagnetic transition in the random layer model, where $g(z)$ performs a random walk.

If positive values of $t$ dominate, so that at $z \to \pm \infty$ the potential $g$ diverges as $\pm |z|$, respectively, then the profile relaxes towards the high-temperature fixed point $\varepsilon = 1$. Similar relaxation to $\varepsilon = -1$ occurs for mostly negative $t$; the two can be combined into the scaling form $\varepsilon = \pm 1 \mp q^2 \mathcal{E}_\pm (z) + o(q^2)$, where

$$\mathcal{E}_\pm = \frac{1}{2} \int_{-\infty}^{z} dz_1 \int_{z}^{+\infty} dz_2 e^{\mp [g(z_2) - g(z_1)]}.$$  \hspace{1cm} (6)

The scaling dimensions describing this \textit{leading irrelevant} behavior at the noncritical fixed points are evidently $\omega_z = 0$, $\omega_\varepsilon = 2$.

If $t(z)$ is mostly positive at $z > 0$ and mostly negative at $z < 0$, so that $g$ has a global minimum around $z = 0$, one finds a nontrivial fixed point

$$\mathcal{E}(y) = -1 + 2 \int_{-\infty}^{y} e^{-g(z)} dz / \int_{-\infty}^{+\infty} e^{-g(z)} dz$$  \hspace{1cm} (7)

scaling with $\omega_z = \omega_\varepsilon = 0$. It describes an interface between the low-temperature phase on the left and the high-temperature phase on the right; note that inversion of this solution, $z \to -z$, implies inverting sign of $g$. In fact, by choosing finite instead of infinite limits of the integrals in (6), (7) one still obtains a local solution to (1); those local solutions will be used below in analyzing the case of a generic, sign indefinite $t(z)$.

The remaining fixed point profiles describe response of a critical system to surface/interface perturbations. The choice of $\omega_z = 1/a > 1$, $\omega_\varepsilon = 0$ yields a solution
\( \mathcal{E}(y) = (1 + A^{-2} y^{2a})^{-1/2} \)  

(8)

describing local, \( \varepsilon_q(z) = t(z)/(t^2(z) + q^2)^{1/2} \), response to a power-law tail \( t(z) = Az^{-a} \).

Scaling in this case is somewhat spurious: the local dependence of \( \varepsilon_q \) on \( t \) is realized whenever the source \( t \) varies slowly on the scale of the local correlation length \( \xi(z) = t^{-1}(z) \), i.e. \( t^{-2} t \ll 1 \). This condition, bound to fail near every zero of \( t \), yields \( a < 1 \) for power-law sources \( t \propto z^{-a} \). Physically it implies that the essential correlations decay faster than the bond strength changes, therefore any physical property can be calculated by simply adding contributions from quasihomogeneous regions. The marginal value \( a = 1 \) leads one to the scaling dimensions \( \omega_z = 1, \omega_\varepsilon = 0 \) of the uniform critical model. Although an explicit solution of the fixed-point equation

\[
[\mathcal{E} - \frac{1}{4} \ddot{\mathcal{E}}][1 - \mathcal{E}^2 + \frac{1}{4} \mathcal{E}^2]^{-1/2} = q^{-1} t(y/q)
\]

(9)

for \( q^{-1} t(y/q) = A/y \) is not available at the moment, presumably such solution exists for any value of the dimensionless amplitude \( A \); interesting properties of this line of fixed points are discussed in [7]. Besides \( t \propto z^{-1} \), the right hand side of (9) is \( q \)-invariant for \( t(z) = 0 \) and \( t(z) = g_0 \delta(z) \); the corresponding fixed point profiles are

\[
\mathcal{E}_s = \text{const } e^{\pm 2y}; \quad \mathcal{E}_d = \tanh(g_0) e^{-2|y|}.
\]

(10)

The first one describes a surface of a critical half-plane in the absence of long range perturbation in the bond strengths, including \( t \propto z^{-a} \) with \( a > 1 \) [7]. Adding two of these half-plane solutions yields \( \mathcal{E}_d \) describing response of a critical system to a defect line [3].

These fixed points allow for a compact description of a general case of an interface geometry [3]. In the most generic case the interface separates two noncritical half-spaces characterized by temperature fields \( t_1, t_2 \). Only the relative sign of the \( t_1 \) and \( t_2 \) turns out to matter then: \( t_1 \) and \( t_2 \) of the same sign inevitably lead to profiles flowing into one of the uniform fixed points (6); opposite signs of the temperature fields, on the other hand, lead to the flow into the nontrivial fixed point (7). This discontinuous change in the form of the profile as one of the half-planes passes its critical point is at the origin of the surface latent
specific heat found in the exact solution of the half-infinite model \[4,6,3\]. At criticality of one of the half-planes the flow can result in one of three fixed points, determined by the range of the surface perturbation in the \(t\)-field, as explained above and in agreement with the analysis in \[7\]. Finally, when both half-planes go critical simultaneously the total strength of the bond perturbation in the interfacial region, as encapsulated in the amplitude \(g_0 = 2 \int t \, dz\) of the \(\delta\)-function, determines which of the line of fixed points \(\mathcal{E}_d\) (10) attracts the flow.

An insight into the nature of some of these fixed-point profiles is provided by the exact equivalence \[9,3\] between each \(q\)-sector of an LPI model and a fictitious one-dimensional classical Ising chain at temperature \(T_{d=1} \sim |\ln q|^{-1}\) and nonuniform reduced magnetic field \(H_{d=1}(z)/k_B T_{d=1} \sim t(z)\). The energy density components \(\varepsilon_q\) map onto the magnetization density of the corresponding \(q\)-chains. The low-\(q\) limit of the planar model corresponds to the low-temperature limit of the chain. The latter is known to be determined by the statistics of a dilute gas of pairs of antiparallel spins which I will call kinks below. A “spin down-spin up” kink, to which orientation \(\sigma = 1\) will be assigned, has to be followed by an “up-down” one, \(\sigma = -1\), etc. The energy of a kink at position \(z\) along the \(q\)-chain is a sum of the cost of creating the kink, \(\ln(1/q)\), and of interaction with magnetic field, \(\sigma g(z)\), leading to the Boltzmann factor \(q \exp(-\sigma g)\). Here the additive constant in the definition of the potential \(g\) is arbitrary but has to be the same for all kinks. One can see now that (7) represents a single kink localized near a global extremum of \(g\). The uniform fixed points naturally correspond to the chain either fully magnetized in one of the two possible directions, \(\varepsilon = \pm 1\), or maintaining zero average magnetization, \(\varepsilon = 0\), at \(T_{d=1} = 0\). The low-\(q\) corrections to these states represent a background of thermally excited single kinks in (4), and pairs of kinks in (6). Other fixed points do not have so simple interpretation, as kinks strongly interact with each other there.

None of the fixed points considered so far addresses directly the situation in which \(t(z)\) has more than one zero, so that \(g(z)\) has many maxima and minima. A crucial insight is provided by consideration of the simplest system with two boundaries. In the present formalism a strip of width \(L\) is represented by \(t(z) = t_1\) at \(|z| < L/2\), surrounded by
At $t > 0$ the energy profile is asymptotically flat, but at $t_1 < 0$ and for sufficient thick films, $|t_1|L \gg 1$, the contradiction between the tendency to ordering within the film and the absence of any order outside of it is resolved by creation of a pair of kinks separating “cool” interior from the “hot” background. Formally a solution is obtained by matching two kink solutions (7) of opposite orientations with three noncritical solutions (6) by choosing appropriate integration constants in those. This construction collapses, however, when $q$ is decreased past $\xi_{\parallel}^{-1} \propto e^{qL|t_1|}$. In the kink picture this comes naturally: the kink-antikink pair is annihilated as soon as the “self-energy” of the pair $2|\ln q|$ exceeds the potential difference $|g(L/2) - g(-L/2)| = 2|t_1|L$ supporting the pair. Physically, the exponential dependence of the crossover scale $\xi_{\parallel}$ on $|t_1|L$ is a signature of the one-dimensional nature of the large scale fluctuations in the film (recall $\ln \xi \propto T^{-1}$ in a classical Ising chain): long range order in a strip of finite width is lost due to activation of two-dimensional domain walls running across the film; the Boltzman factor corresponding to creation of a pair of these walls is $\exp[-2\Sigma(T)L/k_B T]$, where the free energy per unit length of the wall, $\Sigma$, happens to be given by $|t_1|$ in this formalism.

I conjecture now that this mechanism of creation and annihilation of pairs of kinks at maxima and minima of $g(z)$ defines the asymptotic RG flow for a generic temperature field $t(z)$: at a given small $q$ a solution can be constructed by matching pieces of (6) of different signs with the kink-solutions (7). A pair of kinks is stable while these kinks are separated by a potential difference $\Delta g > |\ln q|$; the pair is annihilated at smaller $q$’s. This scenario correctly describes intermediate-scale behavior in the exactly solvable periodic LPI superlattice. Because the fluctuations of potential $g$ in the periodic model are strictly bounded, the critical flow is ultimately attracted by the uniform critical fixed point (4). On the other hand, a random, short range correlated $t(z)$ gives rise to unbounded fluctuations of the random walk type: $\overline{\Delta g^2(z)} = D|z| + o(z)$, with overbar standing for disorder average. Consequently, at a given $q$ the typical size of a pair is going to be $\Delta z = D^{-1}|\ln q|^2$, implying anisotropic scaling $\xi_{\parallel} \propto \exp(D^{1/2}L^{1/2})$ at the critical random fixed point; the subscripts $\parallel, \perp$ indicate directions parallel and perpendicular to the layers. Consider now a random multilayer grown
by subsequent deposition of two different magnetic materials: \( t(z) \) takes two values, \( t_1 \) and \( t_2 \), \( t_1 < t_2 \) with probabilities \( p \) and \( 1-p \), respectively. The average \( \bar{t} = pt_1 + (1-p)t_2 \) goes through zero at a certain temperature \( T_c \); elsewhere a linear bias \( \bar{t}z \) has to be added on top of the random walk exhibited by \( g(z) \) at \( T_c \). Crossover from the critical random to one of the noncritical fixed points happens when potential difference \( \Delta g(\xi) = \bar{t}\xi \) coming from the linear part of \( g \) exceeds the typical random fluctuation on that scale, \( (D\xi)^{1/2} \sim \ln \xi \), so that on larger scales \( g \) is mostly monotonic. This consideration gives

\[
\xi_\perp = D\bar{t}^{-2}, \quad \xi_\parallel = \exp(D\bar{t}^{-1}),
\]

in agreement with the identification of the average correlation lengths in [1(a)]; these lengths are different from the typical correlation lengths, as disorder-average of the logarithm of the correlation function results in \( \bar{\xi} \propto \bar{t}^{-1} \). Although, for instance, at \( \bar{t} > 0 \) the overall positive slope of \( g \) dominates at scales larger than \( \xi \), sufficiently long sequences of \( n \geq |\ln(q)|/|t_1| \) layers of pure low-temperature component occur with small but nonzero density \( p^n \). The associated rare fluctuations in the slope of the potential keep a dilute system of large scale kink pairs from annihilation at any \( q \). First appearance of these large scale pairs at the critical temperature \( T_{c1} \) of the first component, where \( t_1 \) becomes negative, leads to a Griffiths singularity in the free energy, which is easily estimated in agreement with [1]; naturally, the same argument yields a singularity at \( T_{c2} \). One should note that while the singularity at \( T_c \) depends only on the universal large-scale variation, \( \Delta g \propto z^{1/2} \), the essential singularities are governed by the tails of the distribution; if the distribution of \( t(z) \) is Gaussian the singularities are pushed all the way to \( T = 0, \infty \).

This picture is easily generalized to the cases of long-range correlated random and quasiperiodic LPI models. In the first case, the main difference comes with the anomalous scaling dimension \( x_g > \frac{1}{2} \) describing the fluctuations \( \Delta g(z) \propto z^{x_g} \) at criticality, \( \bar{t} = 0 \). The correlation lengths then diverge as \( \xi_\perp \propto t^{-\nu_\perp}, \xi_\parallel \propto \exp[\text{const } t^{-\bar{\nu}_\parallel}] \), with \( \nu_\perp = 1/(1-x_b), \bar{\nu}_\parallel = x_b/(1-x_b) \). On the other hand, if a quasiperiodic one-dimensional binary lattice is constructed by projecting from a strip of finite width cut out of a two-
dimensional lattice \[1\], then \(g(z)\) can be obtained by a similar projection and turns out to be confined within a strip of finite width around the average \(g \propto t z\). Thus critical behavior in this “Fibonacci” multilayer is governed by the pure Ising fixed point (4). Note that the amplitudes of the long wave length harmonics \(t_k \exp(ikz)\) of \(t(z)\) in the Fibonacci sequence are bounded by \(t_k = O(|k|)\); in order for a quasiperiodic sequence to extrapolate between periodic and random behavior, like it was found in \[1\] for a quantum quasiperiodic XY-chain, the amplitudes have to go to zero slower than \(|k|\) so as to generate unbounded fluctuations in the potential \(g\).

In conclusion, an exact functional real space renormalization group flow has been set up and studied for general layered planar Ising models. The RG scheme allows to separate relevant and irrelevant features of a wide class of systems, leading to the classification of various types of critical behavior based on simple basic characteristics, such as the asymptotic variation of the thermal potential \(g = 2 \int t dz\). The surface and random geometries have been analyzed within a single framework leading to a new physical picture of the criticality in a general disordered LPI model: At any finite momentum transfer \(q\) along the layers the system behaves as an alternating sequence of domains of the high- and the low-temperature phases. Having only one infinite dimension, the domains undergo an infinite coarsening as \(q\) decreases. The mechanism of coarsening is activation of linear defects across the finite widths of the domains, hence the exponential scaling (11) at the random criticality. The large fluctuations in the bond strengths underlying the domain structure in this formalism, must be essentially similar to those playing central role in the RG approach of [1(a)].

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