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Extremal statistics in the energetics of domain walls

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We study at $T=0$ the minimum energy of a domain wall and its gap to the first excited state, concentrating on two-dimensional random-bond Ising magnets. The average gap scales as $\Delta E_1 \sim L^\theta f(N_z)$, where $f(y) \sim [\ln y]^{-1/2}$, θ is the energy fluctuation exponent, L is the length scale, and N_z is the number of energy valleys. The logarithmic scaling is due to extremal statistics, which is illustrated by mapping the problem into the Kardar-Parisi-Zhang roughening process. It follows that the susceptibility of domain walls also has a logarithmic dependence on the system size.

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The energy landscapes of random systems are often assumed to be described at low temperatures by scaling exponents that follow from the behavior of the ground states. In renormalization group (RG) language this means that temperature is an irrelevant variable. In most quenched random systems, the energy landscape contains many low-lying metastable minima separated by high barriers. Examples can be found in the realm of random magnets, the most famous one being spin glasses [1]. The dynamical behavior at finite temperatures, as a result of a temperature change or the application of an external field, will naturally depend on the associated barriers and energy differences between the minima.

It is often assumed that energy differences or barriers between configurations (δE) relate to the length l involved by a scaling relation $\delta E \sim l^\theta$, where θ is an energy fluctuation exponent. It measures the dependence of the first nonanalytic correction to the ground state or free energy on the length scale. Here we show that, for extended manifolds, or Ising magnet domain walls (DW's) [equivalent to directed polymers (DP's) in 1+1 dimensions], the energy difference between the ground state energy and the next state (the "first excited state") follows from *extremal statistics*. This is due to the fact that, usually, one can assume that the energy landscape, at large enough scales, consists of many *independent* valleys. Finding the gap between the minimum state and the second-most favorable state is then a straightforward extremal statistics problem, as is the simpler one of the minimum of all the independent valley energies. The extreme statistics leads to logarithmic factors in the gap and minimum energies, which we also show by numerical calculations. The same result can also be applied to other disordered systems, where the energy landscape of DW's can be reduced to a one-dimensional form. We also interpret the results in the language of kinetic roughening, since DP's map into the Kardar-Parisi-Zhang (KPZ) equation of growth [2–4]. Finally, as an application we show that the extremal statistics scaling shows up in the *susceptibility* of DW's.

Here we consider elastic manifolds at $T=0$ with quenched short-range, e.g., pointlike defects, randomness, and in $d=(D+n)$, $n=1$ dimensions, in which D is the di-

mension of the manifolds and d is the dimension of their embedding space. The continuum Hamiltonian for such an elastic manifold is

$$\mathcal{H} = \int \left[\frac{\Gamma}{2} \{ \nabla z(\mathbf{x}) \}^2 + V_r(\mathbf{x}, z) \right] d^D \mathbf{x}, \quad (1)$$

where $z(\mathbf{x})$ is the height of the interface and \mathbf{x} is the D -dimensional internal coordinate of the manifold. The first term in the integrand is the elastic contribution, with the corresponding surface stiffness Γ of the interface, and the second term comes from the random potential. For random manifolds we use quenched random bond (RB) disorder, which means that the random potential is delta point correlated, i.e., $\langle V_r(\mathbf{x}, z) V_r(\mathbf{x}', z') \rangle = 2D \delta(\mathbf{x} - \mathbf{x}') \delta(z - z')$. The geometric behavior of the manifold is characterized by $w^2 = \langle [z(\mathbf{x}) - \overline{z(\mathbf{x})}]^2 \rangle \sim L^{2\zeta}$, where L is the linear size of the system and ζ is the corresponding roughness exponent. At low temperatures in 1+1 dimensions, due to the equivalence of DP's in random media [2,3] to the KPZ equation, the exact roughness exponent reads $\zeta=2/3$ [2–4]. In higher dimensions the functional RG approach gives the approximate expression $\zeta \approx 0.208(4-D)$ [5] for RB DW's. Since the width of a manifold grows as L^ζ , it is expected that the number of independent valleys [6,7] is proportional to $N_z \sim L_z/L^\zeta$. At $T=0$ the total average minimum energy $\langle E_0 \rangle$ of an elastic manifold is equal to its free energy and grows linearly with the manifold area L^D , and its fluctuations scale as $\Delta E = \langle (E_0 - \langle E_0 \rangle)^2 \rangle^{1/2} \sim L^\theta$, where $\theta = 2\zeta + D - 2$ [8].

Let us now analytically derive the scaling of the "extreme statistics" contributions to the lowest minimum E_0 , and the gap between two lowest minima, $\Delta E_1 = E_1 - E_0$. We consider the case of many independent valleys in the landscape $N_z > 1$, which means that the DP's can have an arbitrary starting or end point, and that $L_z > L^\zeta$. For the "single valley" boundary condition case (one end of the manifold fixed), it is known numerically that near its mean the distribution is Gaussian [9]. Hence we draw the energies E from the distribution

$$P(E) = k \exp \left\{ - \left(\frac{|E - \langle E \rangle|}{\Delta E} \right)^\eta \right\}, \quad (2)$$

where $\langle E \rangle \sim L^D$ is the average energy of the manifold, $\Delta E \sim L^\theta$ measures its fluctuations, and k normalizes the integral so $k \sim 1/L^\theta$. The exponent η is not constant [9,3]. Near the peak, $\eta=2$. In the low energy tail numerical simulations indicate that $\eta_- \approx 1.6$, while in the high energy tail the best estimate is $\eta_+ \approx 2.4$ [9]. At this stage we allow η to be variable, but note that it is the behavior near the mean and the *low energy tail* which is the most important in this calculation. In a system with $N_z \sim L_z/L^\xi$ independent local minima, the probability that the global minimum has energy E is given by

$$L_{N_z}(E) = N_z P(E) \{1 - C_1(E)\}^{N_z - 1}, \quad (3)$$

where $C_1(E) = \int_{-\infty}^E P(\epsilon) d\epsilon$ [10]. The gap ΔE_1 follows similarly. Its distribution, $G_{N_z}(\Delta E_1, E)$ is given by

$$G_{N_z}(\Delta E_1, E) = N_z(N_z - 1)P(E)P(E + \Delta E_1) \times \{1 - C_1(E + \Delta E_1)\}^{N_z - 2}. \quad (4)$$

$G_{N_z}(\Delta E_1, E)$ is the probability that if the lowest energy manifold has an energy E , then the gap to the next lowest energy level is ΔE_1 . The average value of the global minimum is given by

$$\langle E_0 \rangle = \int_{-\infty}^{\infty} E L_{N_z}(E) dE, \quad (5)$$

which is not analytically integrable. The typical value of the lowest energy may be estimated using an *extreme scaling* estimate. It follows from the fact the term inside the $\{ \}$ in Eq. (3) becomes unity if C_1 is small enough. This has proven useful in other contexts, for example breakdown of random networks, and here reads [11]

$$1/kN_z P(\langle E_0 \rangle) \approx 1 \quad (6)$$

which yields

$$\langle E_0 \rangle \approx \langle E \rangle - \Delta E \{\ln(N_z)\}^{1/\eta}, \quad (7)$$

where $\Delta E \sim L^\theta$.

To estimate the typical value of the gap, we use, similarly to Eq. (6),

$$1/k^2 N_z(N_z - 1)P(\langle E_0 \rangle)P(\langle E_0 \rangle + \langle \Delta E_1 \rangle) \approx 1, \quad (8)$$

which, with Eq. (7), and the fact that $|\langle \Delta E_1 \rangle| \ll |\langle E_0 \rangle|$, yields

$$\langle \Delta E_1 \rangle \approx \frac{\Delta E^\eta}{\eta(\langle E \rangle - \langle E_0 \rangle)^{\eta-1}} \approx \frac{\Delta E}{\eta \{\ln(N_z)\}^{(\eta-1)/\eta}}. \quad (9)$$

We thus find that, in addition to the usual sample to sample variations in the energy ($\Delta E \sim L^\theta$), there is a slow reduction in the gap which scales as $\{\ln(N_z)\}^{-(\eta-1)/\eta}$, provided $N_z > 1$. Our case is closely related to the *weakly broken replica symmetry* [12] of DP's; also see Ref. [13], where the relation between replica methods and extremal statistics is discussed.

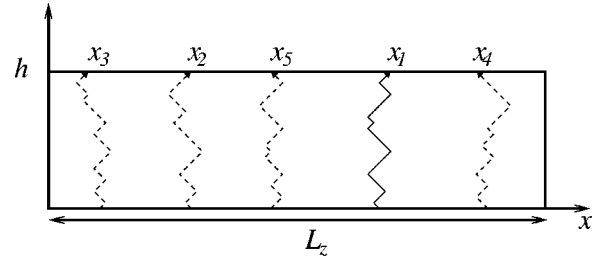


FIG. 1. The relation between DP's and growing interfaces. The KPZ interface is growing, so that h increases and DP's in independent valleys equal the n th fastest arrival times of the interface to a prefixed height h , at x_n , at times $t(x_n)$ in a system with width L_z . The solid line describes the fastest polymer, which ends at x_1 . The dashed lines describe the next fastest polymers.

The (1+1)-dimensional DW maps, in the continuum limit, to the KPZ equation by associating the minimum energy of a DW with the minimum *arrival time* $t_1 \equiv E_0$ of a KPZ surface to height h . The connection is illustrated in Fig. 1 in the limit of many valleys $N_z > 1$. The minimal path of a DW with an end point $z(L)$ is equal to the path by which the interface reaches $h=L$ at a location $x_1 = z$ and at a time $t_1 = E_0$. Thus t_1 attains a logarithmic correction, from Eq. (7), of size $-h^\beta \{\ln(L_z/h^{1/z})\}^{1/\eta}$, where $\beta=1/3$ and $z=3/2$ are now the roughening exponent and dynamical exponent of the KPZ universality class [2]. Now consider the second smallest arrival time t_2 . In the KPZ language of DP's, if the path $x_2(t')$ that gives t_2 is completely independent of the $x_1(t')$ that results in t_1 , then t_2 and x_2 are related to a separate, independent valley of the DP landscape. The *difference* $\Delta t = t_2 - t_1$ is then equal to ΔE_1 of the DW, and likewise obeys extremal statistics, so that $\Delta t \sim h^\beta [\ln(L_z/h^{1/z})]^{-(\eta-1)/\eta}$. For growing surfaces this limit is the *early stages* of growth, in which the correlation length $\xi \ll L_z$, and therefore the arrival times, or DW energies, are independent.

In order to check the scaling behavior of the gap energy [Eq. (9)], we have done extensive exact ground state calculations of elastic manifolds in the two dimensional spin-half RB Ising model, i.e., we take a nearest neighbor Ising model with random but ferromagnetic couplings $J_{ij} > 0$. Calculations are performed by varying both the parallel length L and the height L_z of systems oriented in the $\{10\}$ direction. The DW is imposed by antiperiodic boundary conditions in the z direction at $z=0$ and L_z . The elastic manifold is the interface, which divides the system into two parts, one containing up-spins and the other containing down-spins. At $T=0$ the problem of finding the ground state DW is a global optimization problem, which is solved exactly using a mapping to the minimum-cut maximum-flow problem. The so-called push-and-relabel method solves this problem efficiently, and was extensively discussed elsewhere [14–16].

In order to control the average number of the minima $\langle N_z \rangle \sim L_z/L^\xi$ in a chosen system size, we set the initial position of the interface \bar{z}_0 in a fixed size window at height $\bar{z}_0/L_z \approx \text{const}$. If the ground state interface is originally outside the window, with room only for a single valley, it is neglected, and a new configuration is created. After the original ground state is found, with its energy E_0 , the lattice is

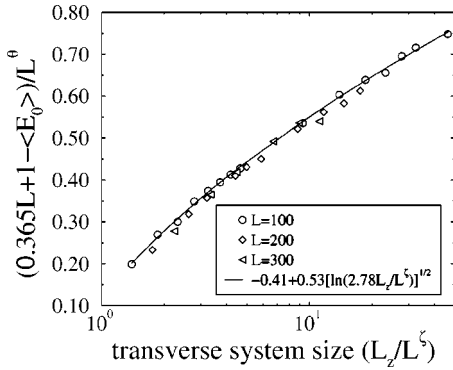


FIG. 2. The scaling of the ground state energy E_0 as a function of scaled transverse system size L_z/L^ζ for the system sizes $L = 100, 200,$ and 300 . The line $-0.41 + 0.53[\ln(2.78L_z/L^\zeta)]^{1/2}$ is a guide to the eye. We have subtracted the expected dependence of $\langle E \rangle$ from $\langle E_0 \rangle$ (see the text). In Figs. 2–4 we use RB disorder, with a $J_{ij,z} \in [0 - 1]$ uniform distribution and $J_{ij,x} = 0.5$. The number of realizations ranges from $N = 500$ for $L = 300$ and $L_z = 500$ to $N = 2000$ for $L = 200$ and $L_z = 600$.

reduced, so that bonds in and above the window are neglected and the new ground state, its E_1 , and the corresponding gap energy ΔE_1 are found. We studied at least $N = 500$ realizations of system sizes up to $L = 300$ and $L_z = 500$. Figure 2 starts the discussion of the numerical data by showing how the ground state energy $\langle E_0 \rangle$ behaves as a function of L and L_z . The scaling result [Eq. (7)] shows that the correction to the energy follows a logarithmic dependence on N_z , which is confirmed in the figure. Note that the extraction of this correction from the data requires an educated guess of how $\langle E \rangle$, the single valley energy, behaves with L . We have used an ansatz $\langle E \rangle \sim aL + b$, with the values of a and b demonstrated in Fig. 2, so that the exponent value $\eta = 2$ corresponds to a Gaussian distribution. Due to the nature of the procedure, it would probably be possible to obtain a reasonable fit for, e.g., $\eta = \eta_-$ as well.

For small sample sizes, $L_z < L^\zeta$ the value of the energy E_0 is affected by confinement. Similarly, the gap is controlled by confinement effects in this limit. When L_z is large there are many independent valleys and extreme statistics effects are important; hence we expect

$$\langle \Delta E_1(L, L_z) \rangle \sim \begin{cases} \tilde{f}(L_z), & L_z \ll L, \\ L^\theta / [\ln(L_z/L^\zeta)]^{(\eta-1)/\eta}, & L_z \gg L \end{cases} \quad (10)$$

where we have used Eq. (9) and $N_z \sim L_z/L^\zeta$. We attempt to collapse the data by using the reduced variables $\langle \Delta E_1(L, L_z) \rangle / L^\theta$ versus L_z/L^ζ for various L and L_z . As seen in Fig. 3 we find a nice agreement with the extreme scaling form, with the ratio $(\eta - 1)/\eta = 1/2$, i.e., by using a Gaussian distribution.

Next we consider the relation of the extremal statistics to the susceptibility of these manifolds. In the D -dimensional case the susceptibility is defined by

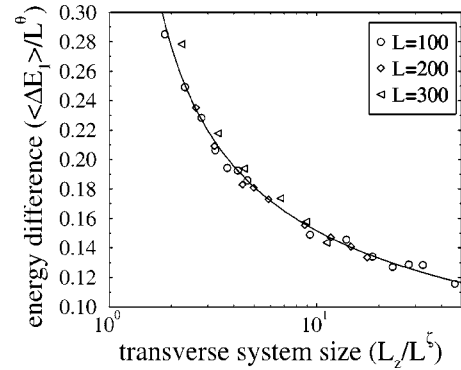


FIG. 3. The scaling function $f(y)$ of the scaled disorder average of the energy difference $\langle \Delta E_1 \rangle / L^\theta$ as a function of scaled transverse system size L_z/L^ζ for the system sizes $L = 100, 200,$ and 300 , each with $\bar{z}_0/L_z \approx \text{const}$. $\theta = 1/3$ and $\zeta = 2/3$. The line has a shape $f(y) = 0.23 \ln(y)^{-1/2}$. The configurations are the same as in Fig. 2.

$$\chi = \lim_{h \rightarrow 0+} \left\langle \frac{\partial m}{\partial h} \right\rangle, \quad (11)$$

where the change in the magnetization of the whole d dimensional system is calculated in the limit of the vanishing external field from the positive side [16,17], and the brackets imply a disorder average. We recently showed that the general behavior follows from a level-crossing phenomenon, which involves an extra potential $V_h(z) = hz$, dependent on the height of the interface, in Hamiltonian (1), and that h is an applied external field to the manifold. In any particular configuration when h is varied, the manifold position changes in macroscopic “jumps” [16], the first one occurring at h_1 .

One may write the susceptibility [Eq. (11)] with the help of the probability distribution of the fields $h_1 P(h_1)$, in the form

$$\chi = \lim_{h \rightarrow 0+} \left\langle \frac{\Delta z}{\Delta h} \right\rangle \approx \left\langle \frac{\Delta z_1}{L_z} \right\rangle \lim_{h \rightarrow 0+} P(h_1), \quad (12)$$

because the magnetization of a system $m(h) \sim \overline{z(h)}/L_z$, and since the distance in the jump between the minima $\langle \Delta z_1 \rangle \sim L_z$ [16], independently of the sample-dependent h_1 . It is expected that a scaling form $P(h_1) \approx \langle h_1 \rangle \bar{P}(h_1/\langle h_1 \rangle)$ applies, and that P remains finite in the limit $h_1 \rightarrow 0$. Next we compare the average susceptibility as a function of the number of valleys N_z to the conjecture that, in the presence of the field, the average gap for the original and excited state follows an extremal statistics form similar to Eq. (9).

The simulations are done again using a fixed height window in which the original ground state without a field is found. After this the external field h is slowly applied by increasing the coupling constant values $J_\perp(z) = J_{\text{random}} + hz$, where J_\perp is perpendicular to the z direction, until the first jump is observed with the corresponding h_1 and Δz_1 . In order to find the scaling relation for the first jump field h_1 , we perform the ansatz $\langle \Delta E_1 \rangle = \langle h_1 \rangle L L_z$, since the field contributes to a polymer energy proportional to L^D ($D = 1$), and

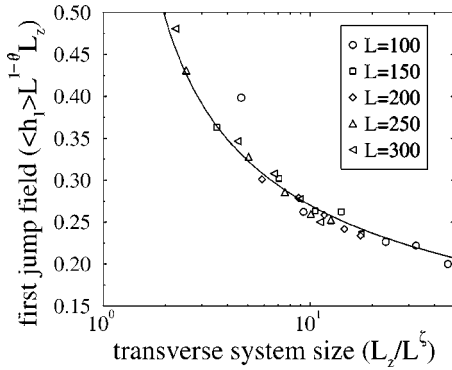


FIG. 4. The scaling function $f(y)$ of the scaled disorder-average of the jump field $\langle h_1 \rangle L^{1-\theta} L_z$ as a function of scaled transverse system size L_z/L^ζ for the system sizes $L=100, 150, 200, 250$, and 300 , each with $\bar{z}_0/L_z \approx \text{const}$. $\theta=1/3$ and $\zeta=2/3$. The line has a shape $f(y)=0.41 (\ln y)^{-1/2}$. Here the number of realizations ranges from $N=500$ for $L=300$ and $L_z=500$ to $N=2600$ for $L=200$ and $L_z=600$.

$L_z \sim \langle \Delta z_1 \rangle$ is the difference in the field contributions hz to the energy at finite h at different average valley heights z_0 and z_1 . Hence

$$\langle h_1(L, L_z) \rangle L L_z \sim L^\theta f\left(\frac{L_z}{L^\zeta}\right), \quad (13)$$

where the scaling function $f(y) = [\ln(L_z/L^\zeta)]^{(\eta-1)/\eta}$. Figure 4 shows the scaling function [Eq. (13)] with a collapse of $\langle h_1(L, L_z) \rangle L^{1-\theta} L_z$ versus L_z/L^ζ for various L and L_z which is again in good agreement with the logarithmic extreme scaling correction. Generalizing to arbitrary dimensions, one has the behavior of $\langle h_1(L, L_z) \rangle \sim L^{\theta-D} L_z^{-1} [\ln(L_z/L^\zeta)]^{-(\eta-1)/\eta}$. For the susceptibility [Eq. (12)], one obtains, using $\langle h_1 \rangle$ for the normalization factor at $P(h_1=0)$,

$$\chi \sim L^{D-\theta} L_z [\ln(L_z/L^\zeta)]^{(\eta-1)/\eta}, \quad (14)$$

and in the isotropic limit $L \propto L_z$, the total susceptibility $\chi_{tot} = L^d \chi$ becomes (when $\eta=2$)

$$\chi_{tot} \sim L^{2D+1-\theta} [(1-\zeta) \ln(L)]^{1/2}. \quad (15)$$

Note that for most random manifolds $1-\zeta > 0$, with the exception of 2D random field Ising DW's for which $\zeta \approx 1$ at large scales [18]; thus the susceptibility does not diverge [19] as the premise $N_z > 1$ does not hold in this case. If the condition $N_z > 1$ is violated, the extreme statistics correction disappears. Thus the extremal statistics of energy landscapes leads to a logarithmic multiplier in the susceptibility [Eq. (15)] of the DW's. This result differs from algebraic forms of scaling [16]; also see Ref. [20].

To conclude, we have considered the average energy differences or ‘‘gaps’’ in the energy landscape of (two-dimensional) elastic manifolds. An extremal statistics argument in a system geometry with many independent valleys shows that the ground state energy and the gap have logarithmic scaling functions, also reproduced with numerical studies. An illuminating connection can be made to Kardar-Parisi-Zhang nonequilibrium surface growth. Finally, we demonstrate that the gap scaling shows up in the susceptibility of random manifolds. This might have implications for flux line lattices in high-temperature superconductors, where a similar problem related to barriers was analyzed with the aid of extremal statistics [21].

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