

Pinning and Roughening of Domain Walls in Ising Systems Due to Random Impurities

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Randomly placed impurities that alter the local exchange couplings, but do not generate random fields or destroy the long-range order, roughen domain walls in Ising systems for dimensionality $\frac{5}{3} < d < 5$. They also pin (localize) the walls in energetically favorable positions. This drastically slows down the kinetics of ordering. The pinned domain wall is a new critical phenomenon governed by a zero-temperature fixed point. For $d=2$, the critical exponents for domain-wall pinning energies and roughness as a function of length scale are estimated from numerically generated ground states.

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Let us consider an Ising ferromagnet (or unfrustrated antiferromagnet) with randomly placed impurities at a temperature below its ordering temperature, T_c . The impurities are assumed to generate random exchange couplings, but not random fields. If the effects of the impurities are sufficiently weak, the system will still order ferromagnetically and we may consider a domain wall separating two domains of predominantly "up" and "down" magnetized spins, respectively. The impurities break the translational symmetry of the system and will tend to pin such a domain wall in certain favorable locations where the exchange couplings are weaker than average.

The Hamiltonian of our system may be written as $H = H_{\text{pure}} + H_{\text{imp}}$, where

$$H_{\text{pure}} = -J \sum_{\langle ij \rangle} s_i s_j \quad (1)$$

is the Hamiltonian of a pure, nonrandom Ising system and H_{imp} contains the effects due to the random impurities. The local equilibrium position of a domain wall in such a random magnet is determined by a compromise between H_{pure} , which tries to minimize the total $(d-1)$ -dimensional area of domain wall, and H_{imp} , which wants the domain wall to deviate from flatness in order to pass through the locations where it has the lowest local energy. The impurity part of our Hamiltonian may be written as

$$H_{\text{imp}} = \sum_{\langle ij \rangle} \Delta J_{ij} s_i s_j, \quad (2)$$

where the $\{\Delta J_{ij}\}$ are randomly distributed. Our results will apply for any distribution of the random couplings ΔJ_{ij} provided that the disorder has only short-range correlations and is not so strong as to destroy the ferromagnetic or antiferromagnetic ordering at low temperatures. This includes the cases of dilution and substitution of negative couplings. In this paper we address the following questions about domain walls in such random-exchange Ising systems: How rough are

they? Do the impurities succeed in pinning them? If so, what are the energy barriers hindering their motion? The last question is important in the understanding of the kinetics of domain growth, which is a process that can be studied experimentally and is discussed at the end of this paper.

Some answers to these questions have recently been obtained for domain walls in *random-field* Ising systems,¹⁻⁴ where $H_{\text{imp}} = \sum_i h_i s_i$ and each h_i is random. Here we are *not* considering random-field or other impurities which couple directly to the local order parameter, but only impurities that couple to the local energy and therefore preserve the up-down Ising symmetry. An example of such a system is a dilute antiferromagnet in *zero* magnetic field. The simple Imry-Ma-type arguments^{1,3,5} which can be used in the random-field case cannot be carried over to this problem because the energy is not a slowly varying function of the domain-wall position.

A summary of this paper and its results is as follows: First, we treat the impurities as a perturbation on a domain wall in a pure system. This analysis shows that in a continuum model, weak impurities will roughen the domain wall even at zero temperature in systems with dimensionality $d < 5$. (On a lattice for $3 < d \leq 5$ the wall may or may not be rough, depending on the strength of lattice effects.) We also show that the pinning energies hindering domain-wall motion diverge at long length scales for $d > \frac{5}{3}$. Secondly, we numerically generate the ground states of domain walls in finite two-dimensional ($d=2$) systems. We find that the domain wall is very rough, with the transverse deviations from a straight line of a segment of interface of length L scaling as L^ζ with $\zeta \approx \frac{2}{3}$, and the pinning energies scaling as L^χ with $\chi \approx \frac{1}{3}$. This scaling behavior shows that the pinned domain wall is a new sort of critical phenomenon, governed by a zero-temperature, strong-pinning fixed point. Presumably a similar behavior, but with different exponents, also occurs for

domain walls in random-exchange Ising systems in $d=3$ and perhaps $d=4$.

We first consider a continuum model of a domain wall in the presence of impurity pinning. The domain wall is assumed to run on average parallel to a reference plane. Let $z(\mathbf{x})$ be the position of the domain wall measured normal to this reference plane at the point specified by the $(d-1)$ -dimensional vector \mathbf{x} . At sufficiently long length scales (long compared to the bulk correlation length)⁶ the relative energy of the domain wall is given by the continuum interface Hamiltonian

$$H_c = \int d^{d-1}x \left[\frac{1}{2} \sigma |\nabla z|^2 + V(\mathbf{x}, z(\mathbf{x})) \right], \quad (3)$$

where σ is the domain-wall stiffness and $V(\mathbf{x}, z)$ is the local domain-wall energy, which is a function of the local impurity density and positions and is random with only short-range correlations. The two terms in this interface Hamiltonian derive from H_{pure} and H_{imp} , respectively. In the pure system $V(\mathbf{x}, z)$ is a constant (which we may set equal to zero) and the ground state of (3) is a perfectly flat domain wall with $z(\mathbf{x})$ constant. For $d > 5$ the presence of weak impurities does not roughen the ground state of the domain wall; the height-difference correlation function

$$G(\mathbf{x}_1 - \mathbf{x}_2) = \langle [z(\mathbf{x}_1) - z(\mathbf{x}_2)]^2 \rangle \quad (4)$$

may be calculated perturbatively to first order in $\langle (\partial V / \partial z)^2 \rangle$ and the result is nondivergent for $|\mathbf{x}_1 - \mathbf{x}_2| \rightarrow \infty$. This calculation is essentially identical to that of Imry and Ma⁵ for systems with $n \geq 2$ component spins, which shows that ferromagnetic ordering in such systems is not destroyed by a weak random field for $d > 4$. The angular brackets in (4) denote averaging over the ensemble of random impurity positions. For $d \leq 5$, on the other hand, infrared divergences are obtained in this perturbative treatment, which suggests that the ground state of (3) is rough. By rough we mean that $G(r)$ diverges for $|r| \rightarrow \infty$. A renormalization-group treatment of this problem, done perturbatively in $\epsilon = 5 - d$, finds that $G(r) \sim |r|^{2\zeta(d)}$, where $\zeta(d) \approx C\epsilon$ for $\epsilon \rightarrow 0$ with $C \approx 0.21$.⁷ Extrapolating this to $d=2$ gives $\zeta \approx 0.63$, which is surprisingly (perhaps fortuitously) close to our numerical result $\zeta(d=2) \approx \frac{2}{3}$, discussed below.

At nonzero temperature the domain wall in the pure system is rough for $d \leq 3$ because of thermal fluctuations.⁶ The Hamiltonian (3) with $V(\mathbf{x}, z) = 0$ is a fixed point of a renormalization-group (RG) rescaling under which the coordinate \mathbf{x} is rescaled to \mathbf{x}/b , and z to $z/b^{(3-d)/2}$. We may then ask if the impurities are relevant or irrelevant at this fixed point. If we start with a weak impurity potential with only short-range correlations (which we approximate with delta func-

tions),

$$\langle V(\mathbf{x}_1, z_1) V(\mathbf{x}_2, z_2) \rangle = \Delta \delta(\mathbf{x}_1 - \mathbf{x}_2) \delta(z_1 - z_2), \quad (5)$$

then simple power counting shows that the impurities are relevant for $d > \frac{5}{3}$, with Δ increasing by a factor of $b^{(3d-5)/2}$ under the RG rescaling. (A more careful momentum-shell integration RG gives the same result.) This shows that for $d > \frac{5}{3}$ the pinning of the domain wall to impurities becomes stronger as one looks at longer length scales and the long-distance behavior is presumably governed by a strong-pinning fixed point.

We now turn to the case $d=2$, where the domain wall is simply a path $z(x)$, so that finding the ground state of the domain wall reduces to an optimal path problem. Let us define $E(x_1, z_1; x_2, z_2)$ as the ground-state energy of a domain wall running from (x_1, z_1) to (x_2, z_2) . Then for any x' between x_1 and x_2

$$E(x_1, z_1; x_2, z_2) = \min_{z'} [E(x_1, z_1; x', z') + E(x', z'; x_2, z_2)]. \quad (6)$$

This equation is the basis of both a transfer-operator approach due to Derrida and Vannimenus⁸ by which we numerically generate ground states, and a real-space RG.

It is instructive to formulate a decimation-type real-space RG for this problem. (Note: We have not actually implemented this RG; we are using it to motivate scaling assumptions.) The function

$$E_a(x; z_1, z_2) = E(x, z_1; x+a, z_2) \quad (7)$$

is distributed according to a functional, $P\{E_a(x; z_1, z_2)\}$, which is assumed to be known. Note that $E_a(x+a; z_2, z_3)$ is independent of $E_a(x; z_1, z_2)$ and has the same distribution. Thus the distribution for $E_{2a}(x; z_1, z_3)$ as obtained with (6) is a kind of nonlinear "convolution" of $P\{E_a\}$ with itself. Let us then rescale the system by a factor of 2 along the x axis and a factor of 2^ζ along the z axis, and rescale energy by 2^χ , defining the renormalized energy function as

$$E'_a(x; z_1, z_2) = 2^{-\chi} E_{2a}(2x; 2^\zeta z_1, 2^\zeta z_2), \quad (8)$$

where the overall additive constant in the energy, which clearly scales as 2^1 , is assumed to be zero. At the fixed point governing the pinned domain wall the resulting distribution of E'_a is identical to $P\{E_a\}$.

In order to investigate this new fixed point we have numerically generated ground states of a lattice version of our model (3) in two bulk dimensions. The lattice Hamiltonian is

$$H_l = \sum_x [J_z |z(x) - z(x+1)| + \Delta J_x(x, z(x))], \quad (9)$$

where z and x are now integers. This is a solid-on-solid model in which the domain wall consists of segments of unit length parallel to the x and z axes with

overhangs forbidden.⁶ The energies of the segments parallel to the x axis, $\Delta J_x(x, z(x))$, are random with no correlations from one location (x, z) to another. The energies of all segments parallel to the z axis are J_z per unit length and not random. We have also examined models with random energies for these segments; as expected by universality, we find no change in the asymptotic scaling behavior. Here we only report results for the simpler model (9).

We use (6) as a transfer operator⁸ to find ground-state energies and positions for long segments of domain walls. For our model (9)

$$E(x, z_2; x+1, z_3) = J_z |z_2 - z_3| + \Delta J_x(x, z_2), \quad (10)$$

so that if we know $E(0, z_1; x, z_2)$ it is a fairly simple operation to generate $E(0, z_1; x+1, z_3)$ by (6). This method has been used to generate exact ground states of domain walls in systems of sizes up to 4000 lattice units long and 2500 wide. If one end of a domain-wall segment of length L is held fixed at, say $(x, z) = (0, 0)$, then the ground state of this segment [subject to the constraint $z(0) = 0$] is given by the minimum of $E_0(L, z) \equiv E(0, 0; L, z)$ with respect to z . Let us define $z_{\min}(L)$ as the value of $z(L)$ in this ground state; $z_{\min}(L)$ is the position of the free end of the domain-wall segment. Since the other end of the segment is held at $z(0) = 0$, the quantity

$$G_0(L) = \langle [z_{\min}(L)]^2 \rangle, \quad (11)$$

is a height difference correlation function closely related to $G(L)$ as defined in Eq. (4). A measure of the pinning energy scale for a domain-wall segment of length L is

$$E_{\text{rms}}(L) = \{ \langle [E_{\min}(L)]^2 \rangle - \langle [E_{\min}(L)] \rangle^2 \}^{1/2}, \quad (12)$$

where $E_{\min}(L) = E_0(L, z_{\min}(L))$ is the ground-state energy with the one end held fixed. By our scaling form (8), we expect that $G_0(L) \sim L^{2\zeta}$ and $E_{\text{rms}}(L) \sim L^\chi$.

In Fig. 1 we show $W(L) = [G_0(L)]^{1/2}$ and $E_{\text{rms}}(L)$ for systems with $J_z = 1$ and ΔJ_x distributed uniformly in $[-\sqrt{12}, \sqrt{12}]$ so that $\langle (\Delta J_x)^2 \rangle = 4$. Two-parameter fits to a power-law form give $\zeta = 0.66 \pm 0.02$ and $\chi = 0.33 \pm 0.01$. We have examined other distributions of ΔJ_x , both two valued and continuous, and find the exponents to be independent (as expected) of the details of the distribution. Since we are dealing with a fairly simple low-dimensional critical phenomenon we suspect that the critical exponents are exactly the simple fractions $\zeta = \frac{2}{3}$ and $\chi = \frac{1}{3}$, but a solid argument for this eludes us.

To obtain a scaling relation between the two exponents ζ and χ , let us consider the average domain-wall energy $\langle E_0(L, z) \rangle$, for a domain wall constrained

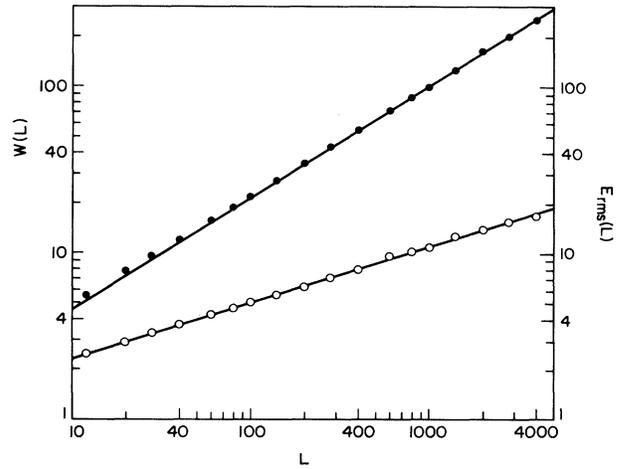


FIG. 1. The root mean square transverse deviation from flatness, $W(L)$, of the ground states of segments of domain wall of length L (upper data), and the energy scale $E_{\text{rms}}(L)$ as defined by Eq. (12) (lower data). Fits with straight lines on the log-log plot give exponent estimates $\zeta = 0.66 \pm 0.02$ and $\chi = 0.33 \pm 0.01$, respectively. The straight lines shown here have the slopes given by the conjectured exact exponents $\zeta = \frac{2}{3}$ and $\chi = \frac{1}{3}$. The deviations from a straight line for small L that can be seen in the data for $W(L)$ are presumably due to corrections to scaling. The statistical errors are less than or equal to (for large L) the size of the points on this graph.

to have slope z/L , for large L and z of order L^ζ . The domain-wall energy per unit length should be analytic in z/L so that $\langle E_0(L, z) \rangle$ may be expanded as

$$\langle E_0(L, z) \rangle = \langle E_0(L, 0) \rangle + \sigma_R z^2 / 2L + O(z^4 / L^3), \quad (13)$$

where σ_R is the domain-wall stiffness at long length scales (fully renormalized). By scaling we also expect that

$$\langle E_0(L, z) - E_0(L, 0) \rangle \approx L^\chi \tilde{E}(z/L^\zeta) \quad (14)$$

for large L , where $\tilde{E}(w)$ is a scaling function. Equating (13) and (14) in the limit $L \rightarrow \infty$, along with the assumption $\zeta \leq 1$ (which is clearly correct here), then yields $2\zeta - \chi = 1$, a simple exponent relation which is certainly consistent with our numerical results. This scaling relation between the exponents ζ for length transverse to the domain wall and χ for relative energy can be readily generalized to other dimensionalities, where it becomes $2\zeta - \chi = 3 - d$.

One reason for interest in the pinning of domain walls is the role that domain-wall motion plays in the kinetics of ordering.⁹ After the system is cooled below its ordering temperature it locally orders into domains separated by domain walls. The average linear domain

size, $R(t)$, grows with time, t , because of domain-wall motion that eliminates the smaller domains, leaving larger ones.⁹ To anneal out the domains of size R requires the movement of domain-wall sections of linear dimension and radius of curvature of order R . If this requires surmounting energy barriers of magnitude $E_0(R)$, then the time scale for this activated process is of order $\exp[E_b(R)/k_B T]$. If $E_b(R) \sim R^\psi$ for large R , as suggested by scaling, then the typical size of the domains left at long times grows as $R(t) \sim (\log t)^{1/\psi}$, as compared to $R(t) \sim \sqrt{t}$ for pure systems.⁹ This domain size, $R(t)$, could be observed as a nonequilibrium correlation length in a scattering experiment.

In order to relate this exponent ψ to those discussed above, ζ and χ , let us follow an argument used by Villain³ for the random-field problem and consider a large, approximately spherical domain of radius R . A section of linear dimension r of the wall of this domain typically deviates from being flat by at least the order of r^2/R . If this section of domain wall is in its ground state (conditioned on its edges being fixed) then it will deviate by order r^ζ from flatness. Thus the roughly spherical domain wall can readily get hung up in a state for which all sections of size $r \lesssim R^{1/(2-\zeta)}$ are in their ground states and the total domain energy can then be lowered only by the movement of larger sections of domain wall inwards. The sections of linear dimension $r_c \sim R^{1/(2-\zeta)}$ that are the easiest to move are roughly flat (if we assume that $\zeta < 1$) so that the energy barriers hindering their motion should scale as r_c^χ . Therefore the barrier $E_b(R)$ for the annealing out of domains of linear dimension R scales with exponent $\psi = \chi/(2-\zeta)$. With our numerical results this gives $\psi \approx \frac{1}{4}$ for the two-dimensional system. For $d \rightarrow 5$ we expect that $\zeta \rightarrow 0$ and $\chi \rightarrow 2$ so that $\psi \rightarrow 1$. Since ψ presumably vanishes at the lower critical dimension of this problem, namely, $d = \frac{5}{3}$, a reasonable interpolation suggests that $1 \geq \psi > \frac{1}{2}$ for $d=3$; the first-order ϵ expansion⁷ gives $\psi(d=3) \approx 0.55$. It will be interesting to see if the logarithmic domain growth, $R(t) \sim (\log t)^{1/\psi}$, that we predict can be observed in nonequilibrium experimental or simulated model systems.¹⁰

The energy barriers $E_b(R)$ that enter in this kinetics-of-ordering argument are barriers against movement of the domain wall by continuous deformation. In our numerical work on the two-dimensional systems we did *not* calculate these barriers; the energy

scale defined by Eq. (12) represents the typical variation of the ground-state energy of a domain-wall segment as one end point (i.e., boundary condition) is moved. Although the end is moved continuously, entire segments of domain wall move discontinuously in this procedure. Thus these energy scales represent lower bounds on the true energy barrier for continuous motion of the entire wall. However, we can also estimate an upper bound by considering, in a hierarchical fashion, motions of shorter and shorter segments of domain wall. This upper bound scales with the same exponent χ , which suggests that $\chi \approx \frac{1}{3}$ is in fact the correct exponent for the true energy barriers for $d=2$.

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Note added.—The transfer operator for the interfacial energies for $d=2$ is closely related to Burger's equation¹¹ with noise. This system has been studied by Forster, Nelson, and Stephen¹² whose results are equivalent to $\zeta = \frac{2}{3}$ and $\chi = \frac{1}{3}$ for our exponents. This will be discussed in future work.⁷

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