Depinning by Quenched Randomness

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An interface attracted by weaker bonds to a wall can be depinned by quenched impurities in the bulk as well as by thermal fluctuations. Exact calculations in two dimensions indicate that the depinning transition with randomness is characterized by a discontinuous specific heat and a quadratic divergence of the localization length. Numerical simulations indicate delocalization by randomness in cases where there is no analogous depinning by thermal fluctuations, e.g., as in an interface bound to a strip of weak bonds in the bulk, or for two attracting interfaces.

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The behavior of an interface close to an attractive wall is important to wetting transitions, and has been extensively studied.[1-5] In two dimensions an exact solution by Abraham[2] indicates that at low enough temperatures an interface is pinned to a wall by weak surface bonds, but at a higher temperature (below the bulk transition temperature) it is unpinned from the surface. The depinning transition is characterized by a discontinuous interface specific heat and a wetting layer whose thickness diverges with an exponent of unity.[2] The nature of the depinning transition in three dimensions is more complex.[3] Here it is pointed out that depinning can be induced by quenched impurities in the bulk, as well as by thermal fluctuations. Randomness is, however, relevant at the transition and modifies the critical behavior. In two dimensions the replica method is used to calculate *exactly* quenched average free energies for interfaces described by the solid-on-solid (SOS) model.[4,5] The depinning transition is still accompanied by a discontinuous specific heat, although the separation from the surface now diverges with an exponent of 2. Numerical simulations indicate that random impurities induce a depinning transition not only from a surface, but also in cases where thermal fluctuations alone are not sufficient to cause a delocalization. The examples studied here are delocalization from a strip of weak bonds in the bulk, and the unpairing of two attracting interfaces. The experimental and theoretical implications of delocalization by quenched impurities in two and more dimensions are discussed.

Abraham[2] originally considered an Ising model on a semi-infinite square lattice, with weak bonds at the surface, and boundary conditions chosen so as to introduce an interface separating up and down domains. However, it was found[4,5] that the transition is not affected by going to the SOS limit, which excludes overhangs and island fluctuations, and is considerably simpler to analyze. Here the SOS model is considered in the presence of random bonds. The interface runs parallel to the x axis on a square lattice with $y \geq 1$, and one end pinned to $y=0$ at $x=1$. At zero temperature, in the absence of random bonds, it stays at $y=1$ for all x to take advantage of the weak surface bonds. At finite temperatures and because of randomness, the interface fluctuates and its configuration is described by the set of integer heights $\{y(x)\}$. The energy cost of each configuration has a contribution $\sum_x \mu(x,y)$ for vertical bonds broken at positions $\{y(x)\}$, and a part $K_x \sum_x |y(x+1)-y(x)|$ from broken horizontal bonds. For simplicity only configurations with $|y(x+1)-y(x)|=0$ or 1 are included (this is not an important restriction at low temperatures), and there is a Boltzmann factor $\gamma=\exp(-K_x)$ for each jump $y(x+1)=y(x)\pm 1$. The bonds on the surface $\mu(x,1)=\mu_s$ are weaker than the bonds in the bulk, which are assumed to be independent Gaussian random variables of mean μ_a and variance σ^2. The total weight $W(x,y)$ of interfaces connecting (0,1) to (x,y) can be calculated recursively by a transfer matrix, $W(x,y)=\sum_{y'}\langle y|T(x)|y'\rangle W(x-1,y')$, with

$$\langle y|T(x)|y'\rangle = \begin{cases} \exp[-\mu(x,y)](\delta_{y,y'}+\gamma\delta_{y,y'-1}+\gamma\delta_{y,y'+1}), & y>1, \\ \exp(-\mu_s)(\delta_{1,y'}+\gamma\delta_{2,y'}), & y=1. \end{cases} \tag{1}$$

In the limit $\gamma \ll 1$, the discrete problem can be replaced by a continuum one with $T(x)=\exp(-\mathscr{H}(x))$, and the "time-$x$" dependent Hamiltonian for a particle in a random potential

$$\mathscr{H}(x) = -\gamma d^2/dy^2 + V_s(y) + \mu(x,y). \tag{2}$$

The surface potential $V_s(y)$ can be represented by an attractive well next to an impenetrable wall. In the absence of randomness, the ground-state wave function is $\psi(y)\sim\exp(-\lambda y)$, with $\lambda=[(\mu_b-\mu_s)-\gamma]/\gamma$. The inverse localization length, $l=1/\lambda$, results from a

competition between the pinning energy $\mu_b - \mu_s$ and the entropy loss due to elimination of paths to $y < 1$ by the surface. The entropy term dominates at high temperatures, and a depinning transition occurs at $\gamma = \mu_b - \mu_s$, with the localization length diverging with an exponent of unity. [For a strip of weak bonds in the bulk, corresponding to a delta-function potential in (2), the entropy loss term is absent and the interface is always localized.[4]] The free energy, corresponding to the ground-state energy of Hamiltonian (2), is $f = \mu_b - 2\gamma - \gamma\lambda^2$. It describes a second-order transition with a discontinuous interface specific heat.[4,5]

With random bonds $\mu(x,y)$, the quenched average free energy is calculated by the replica method $\{[\ln Z]_\mu = \lim_{n\to 0}([Z^n]_\mu - 1)/n\}$, where Z^n corresponds to n replicated interfaces. $[\ldots]_\mu$ denotes random-bond averaging in the text, while an overbar is used in the figures. If m interfaces cross at a bond $\mu(x,y)$, the averaging process

$$[\exp(-m\mu)]_\mu = \exp[-m(\mu_a - \sigma^2/2) + m(m-1)\sigma^2/2]$$

renormalizes the bulk bond energy to $\mu_b = \mu_a - \sigma^2/2$, and introduces a pairwise attraction of magnitude σ^2 between the interfaces. The x-independent transfer matrix is now $T_n = \exp(-\mathscr{H}_n)$, with the n-particle Hamiltonian

$$H_n = n(\mu_b - 2\gamma) + \sum_{\alpha=1}^{n}\left[-\gamma\frac{d^2}{dy_\alpha^2} + V_s(y_\alpha)\right] - \frac{\sigma^2}{2}\sum_{\alpha\neq\beta}\delta(x_\alpha - x_\beta). \tag{3}$$

Since $n(\mu_b - 2\gamma)$ is just an analytic additive term in the free energy, it will be ignored henceforth. First the free energy of an unbound interface (far away from the surface) is calculated. In the absence of the potential the coordinates y_α range from $-\infty$ to ∞, and the ground-state wave function is

$$\psi(y_1, \ldots, y_n) = \exp(-\kappa \sum_{\alpha<\beta} |y_\alpha - y_\beta|),$$

where $4\gamma\kappa = \sigma^2$ ensures the proper discontinuity in the wave function derivative as two particles cross. Note that a new length scale $l_d = \kappa^{-1} = 4\gamma/\sigma^2$, associated with disorder, appears in the problem. As discussed previously[6] in connection with commensurate to incommensurate transitions, new critical behavior is expected at length scales larger than l_d. The quenched average free energy is obtained from

$$[f_0]_\mu = \lim_{n\to 0}(E_n/n) = \lim_{n\to 0}[-\gamma\kappa^2(n^2-1)/3] = \gamma\kappa^2/3. \tag{4}$$

In the bound state, the wave function for any arrangement $1 < y_{P1} < \ldots < y_{Pn}$ corresponding to a permutation P of n particles, is $\psi(y_{P1}, \ldots, y_{Pn}) = \exp(-\sum_{\alpha=1}^{n}\kappa_\alpha y_{P\alpha})$, with $\kappa_\alpha = \lambda + 2(\alpha-1)\kappa$. This function has the proper derivative discontinuities when particles meet, and falls off as $\exp(-\lambda y_{P1})$ close to the surface. (The possibility of more than one particle inside the potential has been ignored. For this assumption and the continuum limit to be valid, in addition to γ, λ and κ must also be much less than unity.) The quenched average free energy of the surface state is given by

$$[f_s]_\mu = \lim_{n\to 0}\gamma[\lambda^2 + 2\lambda\kappa(n-1) + 2\kappa^2(n-1)(2n-1)/3] = -\gamma(\lambda^2 - 2\lambda\kappa + 2\kappa^2/3). \tag{5}$$

The important quantity is the difference in free energies between the free and bound states, i.e., $[f_s]_\mu - [f_0]_\mu = -\gamma(\lambda-\kappa)^2$. The binding free energy is decreased by randomness and goes to zero at $\kappa = \lambda$. Thus the depinning transition can be induced by increasing bond randomness, as well as by thermal fluctuations. The quadratic nature of the free energy indicates a discontinuous interface specific heat through the transition, which is similar to the discontinuity observed when the depinning is induced by thermal fluctuations. However, the quenched average separation of the interface from the wall, calculated from the wave function after some manipulation, is

$$[\langle y\rangle]_\mu = \lim_{n\to 0}\langle n^{-1}\textstyle\sum_\alpha y_\alpha\rangle_n = \int_0^\infty dx\, \kappa x e^{-(\lambda-\kappa)x}/(1-e^{-\kappa x}). \tag{6}$$

For $\kappa \ll \lambda$, $[\langle y\rangle]_\mu = 1/\lambda$ as before, while close to the transition it diverges as $[\langle y\rangle]_\mu \sim \kappa/(\lambda-\kappa)^2$. Therefore, the exponent for the divergence of the localization length changes from 1 in the pure system to 2 in the presence of randomness.

Randomness, in fact, modifies the critical behavior of the wetting transition for dimensions $d > \frac{5}{3}$. This is shown by examining a continuum version of the interface problem in d dimensions. The interface height is now $y(\mathbf{x})$, with $\mathbf{x}$ a $(d-1)$-dimensional vector. The continuum Hamiltonian is

$$\mathscr{H} = \int d^{d-1}x\,[\tfrac{1}{2}\gamma(\nabla y)^2 + \mu(\mathbf{x},y) + V_s(y)], \tag{7}$$

where γ plays the role of the interface tension, $\mu(\mathbf{x},y)$ is related to the randomness, and $V_s(y)$ is the surface potential. Under a rescaling $\mathbf{x} \to \lambda\mathbf{x}$ and $y \to \lambda^\zeta y$, $\gamma \to \gamma\lambda^{d-3+2\zeta}$, and the surface tension remains fixed for $\zeta_0 = (3-d)/2$. This is the exponent for interface roughening in the absence of randomness. The scaling

of randomness obtained from

$$[\delta\mu(\mathbf{x},y)\delta\mu(\mathbf{x}',y')]_\mu=\sigma^2\delta^{d-1}(\mathbf{x}-\mathbf{x}')\delta(y-y')$$

is $\sigma^2\to\sigma^2\lambda^{d-1-\zeta}$ or $\sigma^2\lambda^{(3d-5)/2}$ with use of ζ_0 given above.[7] This implies that randomness is relevant[7] for $d>\frac{5}{3}$ and modifies the roughening exponent ζ. In two dimensions, recent results[6-8] indicate $\zeta=\frac{2}{3}$ with randomness (as compared to $\zeta_0=\frac{1}{2}$). A pinning potential V_s, close to the surface (or from a strip of weak bonds in bulk), behaves as $t\delta(y)$ and also scales as $t\to t\lambda^{d-1-\zeta}$. The similarity in scaling of randomness and the pinning potential is consistent with the results obtained above, i.e., as the relative strengths of these effects is changed, there can be a transition from an interface pinned by the surface to one pinned to the random bonds in the bulk. (Note that the critical dimension of interface delocalization is $\frac{5}{3}$, as opposed to 2 for delocalization of a particle from an attractive potential.) The wetting transition is in a new universality class for $d>\frac{5}{3}$, when randomness is relevant. Indeed the scaling form for t suggests a localization length diverging as $y\sim t^{-\nu}$, with $\nu=\zeta/(d-1-\zeta)$. Although this result is correct for the random and nonrandom examples in two dimensions, its validity in general requires further study.

Since the $n\to 0$ limit of the replica method may introduce complications, it is worthwhile to complement the theoretical results with numerical simulations. For a given realization $\{\mu(x,y)\}$ of randomness the weights $W(x,y)$ are generated recursively from Eq. (1), starting with the interface at the origin $[W(0,y)=\delta_{y,0}]$. The weights are then used to calculate $\langle y\rangle$ for each x, and the quenched averaging is performed by summing over many realizations of randomness. (Note that unlike Monte Carlo simulations, for a given realization the transfer matrix gives exact results.) Figure 1 shows numerical results for $[\langle y\rangle]_\mu$, close to an attractive interface with $z=\exp(\mu_s-\mu_a)=1.4$, $\gamma=0.3$, and for different amounts of randomness. It is numerically convenient to use uniform random variables of width s, rather than Gaussian variables of variance σ^2 ($\sigma^2=s^2/12$). For this reason, and since relatively large values of γ are used, a quantitative comparison with the continuum model cannot be made, although the qualitative behavior is expected to be similar. The solid curves in Fig. 1 correspond to $s=0$, 0.1, 0.2, and 0.3. As the amount of randomness is increased the interface moves away from the wall, and is unpinned by randomness at $s\lesssim 0.3$. The dashed line represents an interface in the nonrandom case ($s=0$), but with $\gamma=0.7$. In this case the depinning is caused by thermal fluctuations. In a log-log plot, asymptotic slopes of $\frac{1}{2}$ and $\frac{2}{3}$ are expected for the unpinned-pure and random interfaces, respectively.[7,8] Although the slope of the solid line in Fig. 1 is larger than the dashed line, neither curve has reached its asymptotic limit.

I also used numerical simulations to study two problems where I was unable to obtain any analytical results. One is that of pinning to a strip of weak bonds in the bulk (instead of on the surface), corresponding to a square-well potential in Eq. (2). In the absence of randomness since the ground-state wave function is always localized, the interface is pinned to the weak bonds. With randomness present the behavior of the interface is studied numerically. The results in Fig. 2 correspond to a strip of attractive bonds of strength

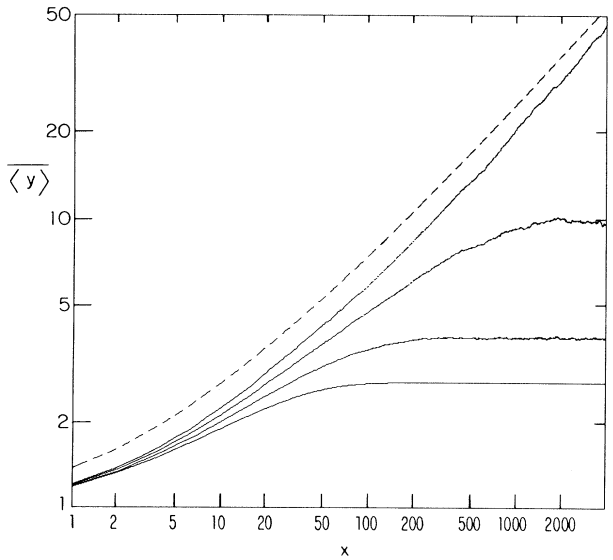

FIG. 1. Fluctuations of an interface from an attracting wall due to impurities. Solid lines correspond to random bonds of widths $s=0$, 0.1, 0.2, and 0.3, respectively, with $\gamma=0.3$. The dashed line corresponds to $\gamma=0.7$ and $s=0$.

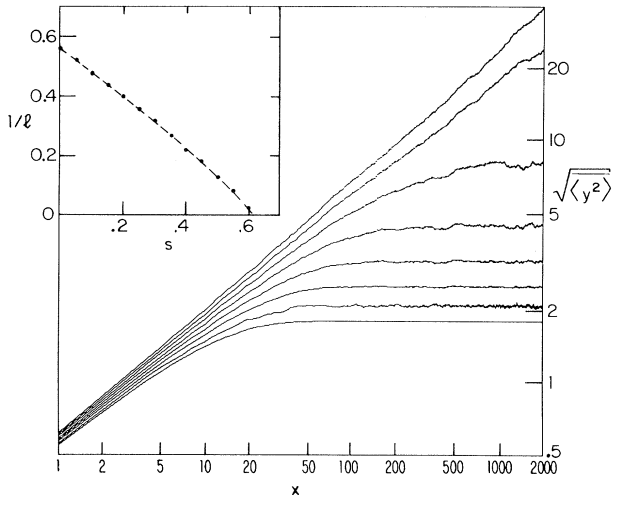

FIG. 2. Delocalization by randomness from an attracting strip at $y=0$. The solid curves correspond to s increasing from 0 to 0.7 in steps of 0.1. The inverse localization length is plotted in the inset.

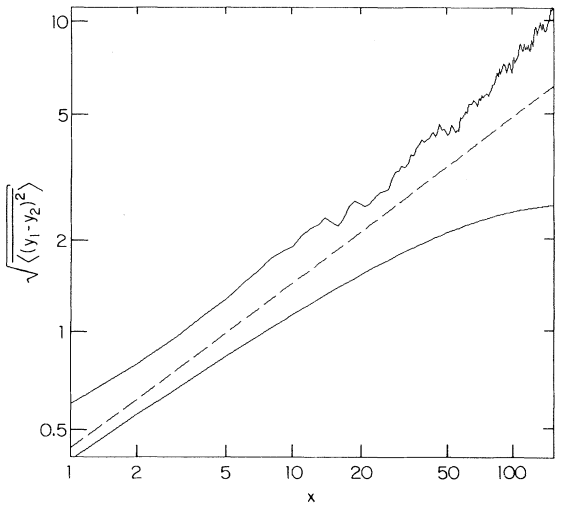

FIG. 3. Unpairing of attracting interfaces (solid lines) by randomness; $s=0$ and 6, respectively. The dashed line shows the separation of repelling interfaces with $s=0$.

$z=\exp(\mu_0-\mu_a)=1.4$ at $y=0$, with $\gamma=0.3$. The interface starts from $y=0$ at $x=0$, and the bulk bonds are uniformly distributed about μ_a in an interval of width s. As s is increased from 0 to 0.7, the interface moves away from the origin and is depinned for large s. It is of course possible that $\{[\langle y^2\rangle]\}^{1/2}$ always asymptotically tends to a large but finite value. However, the inset in Fig. 2 indicates that the localization length probably diverges for $s\sim 0.6$. The delocalization transition is expected to occur when the disorder length $l_d=\kappa^{-1}$ becomes comparable to the localization length in the absence of impurities. The discussion following Eq. (7) suggests that the delocalization transition is probably in the same universality class as the depinning transition studied earlier. The divergence of l from the Fig. 2 inset, however, seems linear rather than quadratic. This discrepancy is not serious if the data points are not in the asymptotic regime. As in the previous figure, much longer interfaces are necessary to examine the true asymptotic behavior.

Yet another delocalization transition of interest is that of two (or generally more) attracting interfaces. Weeks and Chui[4] have proposed that steps on the surfaces of semiconductors provide an experimental realization of such attracting interfaces. Indistinguishable or noncrossing interfaces, such as the steps on a crystal surface, undergo an unbinding transition as temperature is increased (again driven by the gain in entropy). By contrast, distinguishable interfaces that are allowed to cross are always bound, and cannot be unpaired by thermal fluctuations alone. The solid lines in Fig. 3 show the separation of two such attracting distinguishable interfaces ($z=1.1$ on collision) with $\gamma=0.05$ for $s=0$ and $s=6$. (The interfaces start at the same point at $x=0$.) It can be seen that randomness separates the interfaces, and again an unpairing transition probably occurs for $\kappa\sim\lambda$. The dashed line shows the separation of repelling interfaces ($z=0.9$) in a pure system, and it has a smaller slope than the solid line for $s=6$ as expected. (A similar unpairing is also expected for indistinguishable interfaces). It would be interesting to look for such impurity-driven unpairing transitions experimentally.

To summarize, it was shown that the depinning transition can be induced by randomness, as well as by thermal fluctuations. Exact calculations in two dimensions indicate that the depinning transition with randomness belongs to a new universality class, with a discontinuous specific heat and a quadratic divergence of the localization length. Indeed the scaling of interface fluctuations with impurities is described by a new critical point for dimensions $\frac{5}{3}<d<5$.[7] This new scaling also modifies the commensurate to incommensurate[6] and wetting (depinning) transitions that are directly driven by interface fluctuations. Numerical simulations indicate that bulk randomness is also capable of inducing delocalization in cases where thermal fluctuations alone are not sufficient, e.g., interfaces bound to strips of weak bonds in the bulk, or a pair of distinguishable attracting interfaces. The unpairing transition may have an experimental realization in attracting steps on a semiconductor surface.[4] Further study of the unpairing of attracting interfaces can also shed light on how randomness modifies fluctuations and criticality. In a three-state Potts model, for example, a 1-3 interface can be regarded as indistinguishable attracting 1-2 and 2-3 boundaries. Since randomness tends to unpair such boundaries, the random Potts interface will be thicker (wetter) than the pure one, and the vanishing of the surface tension is expected to be different.

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