Disorder-Driven Critical Behavior of Periodic Elastic Media in a Crystal Potential

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A lattice model of a three-dimensional periodic elastic medium at zero temperature is studied with exact combinatorial optimization methods. A competition between pinning of the elastic medium, representing magnetic flux lines in a superconductor or charge density waves in a crystal, by randomly distributed impurities and a periodic lattice potential gives rise to a continuous roughening transition from a flat to a rough phase. A finite size scaling analysis yields the critical exponents $\nu \approx 1.3$, $\beta \approx 0.05$, $\gamma/\nu \approx 2.9$ that are universal with respect to the periodicity of the lattice potential. The small order parameter exponent is reminiscent of the random field Ising critical behavior in 3D.

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A number of materials possess an instability towards the formation of a periodically modulated structure in space below a particular temperature. Prominent examples are charge-density wave systems [1], where a Peierls instability leads to a state with periodically varying charge modulation, or magnetic flux lines in the mixed phase of high-temperature superconductors [2], where the long-range interaction among the lines results in the formation of the Abrikosov flux-line lattice. Other systems forming such periodic structures are spin density waves in anisotropic metals, polarization density waves in incommensurate ferroelectrics, and mass density waves in superionic conductors [3].

Usually the periodicity $\mathbf{q}$ of this state of broken translational invariance is incommensurate with the underlying crystal lattice, but if $\mathbf{q}$ and a reciprocal lattice vector $\mathbf{k}$ become commensurate ($\mathbf{q} \approx \mathbf{k}/p$), where p is a rational number, the density wave locks in at this wave vector. If fluctuations — either thermal or induced by impurities, i.e., quenched disorder — are weak, these systems are then in a *flat* phase that can be quantified by an order parameter reflecting the broken symmetry. Deviations of the local density from the perfect periodic structure can be measured by a displacement field $\phi(\mathbf{r})$, which shows long-range order in the flat phase. When the fluctuations become too strong, this long-range order vanishes at a roughening transition and the system enters a *rough* phase in which the displacement-displacement correlations $\langle[\phi(\mathbf{r}) - \phi(\mathbf{0})]^2\rangle$ diverge with the distance r.

In the presence of quenched disorder this roughening transition is driven by the competition between two pinning forces acting on the periodically modulated flat phase: one coming from the underlying lattice potential preferring long-range order and the other by the point impurities tending to destroy it. The universality class of this transition in the experimentally most relevant case of three space dimensions (3D), its critical exponents, and the scaling laws have not been directly scrutinized up to now and are the topic of this Letter. Thermal fluctuations are expected to be (dangerously) irrelevant at the roughening transition [4], and the critical behavior at the transition should be dominated by a zero temperature fixed point analogous to random field critical behavior [5]. Hence the universal properties of the roughening transition at *finite* temperatures are expected to be identical to the one at *zero temperature* and the critical exponents can, in principle, be extracted numerically by exact ground state calculations [6,7], which is the method that we use here.

The model Hamiltonian that captures the universal properties of the roughening transition under consideration should contain the following features: It should be formulated in terms of a (scalar) displacement field $\phi(\mathbf{r}) \in (-\infty, +\infty)$, an elastic energy term $\frac{\gamma}{2}(\nabla\phi)^2$ as the first order (elastic) approximation of the interaction energy arising from small deformations of the flat state $\phi(\mathbf{r}) = \text{const}$, a periodic potential $V_{\text{per}}(\phi) = V_{\text{per}}(\phi + 2\pi/p)$, where p is rational, modeling the crystal lattice, and a random potential $V_{\text{rand}}(\phi)$ mimicking the effect of impurities, which should be invariant under the global shift of the whole displacement field $\phi \to \phi + 2\pi$. The commensurability parameter p entering the periodic potential is integer for the lock-in state and is given by the ratio of lattice constant of the elastic media with respect to that of the underlying periodic potential. The following Hamiltonian fulfills these requirements [3,4]:

$$\mathcal{H} = \int d^d\mathbf{r} \left[\frac{\gamma}{2} |\nabla\phi|^2 - \upsilon \cos(p\phi) + \eta \cos(\phi - \varphi) \right], \quad (1)$$

where $\varphi(\mathbf{r})$ are independent quenched random variables uniformly distributed on $[-\pi, \pi]$ and γ, υ, and $\eta(\mathbf{r})$ denote the elastic constant, the periodic potential strength, and the random potential strength, respectively. The underlying elastic approximation for this model is valid as long as disorder induced topological defects do not proliferate. In 2D this actually happens [8], but in 3D the elastic medium is stable for weak disorder [9].

For $v = 0$, the Gaussian variational and the functional renormalization group (FRG) calculations [10,11] and numerical studies [12] show that the system is in the elastic glass phase, corresponding to a zero-temperature fixed point, at all temperatures. The elastic glass phase in 3D is characterized by diverging fluctuations

$$G(\mathbf{r}) = \overline{\langle[\phi(\mathbf{r}_0 + \mathbf{r}) - \phi(\mathbf{r}_0)]^2\rangle} \simeq 2A \ln|\mathbf{r}| \quad (2)$$

at large distances with a universal coefficient A. The overbar denotes the disorder average and $\langle\cdots\rangle$ denotes the spatial average over $\mathbf{r}_0$ and the thermal average.

A simple scaling argument [4,13,14] shows that for $d > 2$ the flat phase ($\phi = 2\pi n/p$, where n is a fixed integer) is stable as long as the disorder is weak enough: For vanishing disorder $\eta = 0$ an excitation $\phi \to \phi + 2\pi/p$ over a terrace of linear scale ξ costs an elastic energy of the order of ξ^{d-1}, whereas for nonvanishing disorder the same excitation could gain energy of order $\xi^{d/2}$. Thus for $d > 2$ the elastic energy loss will dominate over weak disorder and the ground state stays flat. Only a strong enough disorder will drive the periodic medium into the rough phase. This disorder-driven roughening transition was first [15] studied within a variational theory in [16] for the elastic manifold case, where a first order transition was found, whereas the FRG method used in [4] predicted a continuous roughening transition for $p > p_c(d) = 6/(\pi\sqrt{\epsilon})$ with $\epsilon = 4 - d$ at finite disorder strength that is determined by a zero-temperature fixed point. The order parameter exponent β and the correlation length exponent ν were given to leading order in a double expansion in ϵ and $\mu = p^2/p_c^2 - 1$ by

$$\nu^{-1} = 4\mu, \qquad \beta/\nu = (\pi^2/18)\epsilon\,. \quad (3)$$

A naive insertion of $d = 3$ and $p_c = 6/\pi$ into these expressions yields values for β and ν that are incompatible with our results which we report now.

We consider a discrete model for the continuum Hamiltonian (1). Because of the periodic potential the elastic medium remains flat on a microscopic length scale with

$$\phi = (2\pi/p)h, \qquad h \text{ integer}\,. \quad (4)$$

Therefore, on a coarse-grained level, the medium can be described by this integer height variable $\{h_\mathbf{x}\}$ representing a $(3 + 1)$-dimensional surface on a simple cubic lattice with sites $\mathbf{x} \in \{1,\ldots,L\}^3$. Creating steps costs elastic energy and the surface is subjected to a random pinning potential. These effects plus the periodic potential are incorporated in the following solid-on-solid (SOS) model Hamiltonian:

$$\mathcal{H} = \sum_{(\mathbf{x},\mathbf{y})} J_{(h_\mathbf{x},\mathbf{x});(h_\mathbf{y},\mathbf{y})}|h_\mathbf{x} - h_\mathbf{y}| - \sum_\mathbf{x} \eta_\mathbf{x} \cos[(2\pi/p)h_\mathbf{x} - \varphi_\mathbf{x}], \quad (5)$$

where the first sum runs over nearest neighbor pairs $(\mathbf{x},\mathbf{y})$ on a simple cubic lattice. The Hamiltonian has to be invariant under a global shift $h \to h + p$, which is inherited from the symmetry under $\phi \to \phi + 2\pi$ of the continuum Hamiltonian (1). Hence we impose a periodicity in the step energies J by $J_{(h+p,\mathbf{x});(h'+p,\mathbf{y})} = J_{(h,\mathbf{x});(h',\mathbf{y})}$. Although various aspects of the microscopic physics of the lattice model (5) and the continuum Hamiltonian (1) might be different, we can expect the roughening transition occurring in both models to be in the same universality class, since both models have identical symmetries. This 3D SOS model is then mapped onto a (3+1)-dimensional ferromagnetic random bond Ising model with an antiperiodic boundary condition in the extra direction, denoted by u [17]. In the ground state the latter induces a 3D interface, identical to the surface we are searching (up to a global shift) that can be determined *exactly* by using a min-cut/max-flow algorithm (see [6,12] for details).

We study the model (5) with $p = 2, 3$, and 4 in finite $L^3 \times U$ lattices with $L \leq 32$. The lattice size in the u direction, U, has to be chosen large enough in order to avoid an interference of the surface with the boundary. Random couplings are assigned to the bonds in a unit cell of size $L^3 \times p$ and they are repeated periodically in the u direction. Then the exact ground state configuration is calculated using a max-flow algorithm. We present numerical results obtained by using the uniform distribution for $0 \leq \varphi_\mathbf{x} < 2\pi$ and $0 \leq \eta_\mathbf{x} < V$ and the exponential distribution, $P(J) = J_0^{-1} e^{-J/J_0}$, for $J > 0$ [18]. The strength of the random pinning potential is denoted by $\Delta \equiv V/J_0$ and we vary this quantity to trigger the roughening transition in our system.

For each p, we measure the magnetizations

$$m_{p,q}(L,\Delta) = \overline{|\langle e^{2\pi i h_\mathbf{x}/q}\rangle|} \qquad (q = 2,3,\ldots) \quad (6)$$

with $\langle(\cdots)\rangle$ and $\overline{(\cdots)}$ denoting the spatial and the disorder average, respectively, in the ground state. Typically the disorder average is taken over 10 000–3000 samples for $L = 4$–32. Note that the order parameter $m = \overline{\langle e^{i\phi}\rangle}$ considered in Ref. [4] corresponds to $m_{p,q=p}$; cf. Eq. (4).

In Fig. 1 we show the magnetization for $p = 2$ as a function of L, which scales at the critical point $\Delta = \Delta_c$ like $m_{p,q} \sim L^{-\beta_{p,q}/\nu}$, where $\beta_{p,q}$ and ν are the order parameter and correlation length exponent, respectively. This scaling is followed best by the data at $\Delta = 2.20$, whereas there is a downward (upward) curvature for $\Delta = 2.23$ (2.17) when plotting $\ln m_{p,q}$ vs $\ln L$. The critical point Δ_c can be directly determined by looking at the effective exponent

$$[\beta_{p,q}/\nu]_L \equiv -\frac{\ln[m_{p,q}(2L)/m_{p,q}(L)]}{\ln 2}\,, \quad (7)$$

which is (asymptotically) independent of system size at the critical point and equal to the critical exponents $\beta_{p,q}/\nu$ (see Table I).

The correlation length exponent is obtained from the scaling behavior near the critical point. Each quantity is a function of L/ξ with the correlation length $\xi \sim |\Delta - \Delta_c|^{-\nu}$ such that the scaling form of the magnetization is

$$m_{p,q}(L,\Delta) = L^{-\beta_{p,q}/\nu}\mathcal{F}((\Delta - \Delta_c)L^{1/\nu}) \quad (8)$$

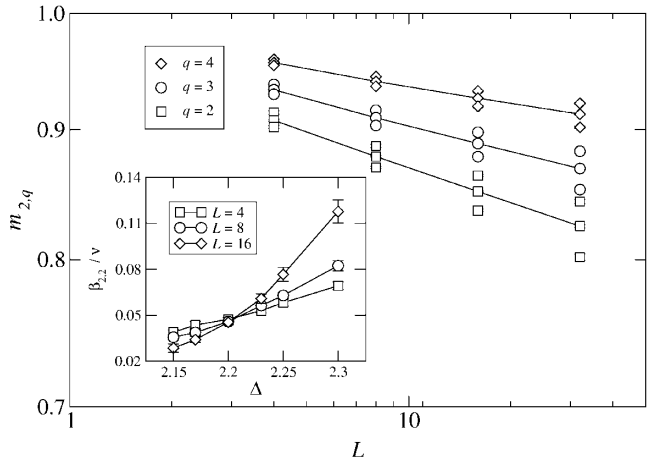

FIG. 1. Magnetizations $m_{p,q}$ ($q = 2, 3, 4$) at $p = 2$ and $\Delta = 2.17$, 2.20, and 2.23 from top to bottom. The data at the critical point $\Delta_c = 2.20$ are connected by solid lines. The inset shows the effective exponents for $m_{2,2}$ [Eq. (7)].

with a scaling function $\mathcal{F}$. Using the values of Δ_c and $\beta_{2,2}/\nu$ estimated previously, we determine the correlation length exponent as the optimal value which yields the best data collapse of $m_{2,q=2}(L, \Delta)$. The estimated correlation length exponent is also listed in Table I and the scaling plot is given in Fig. 2(a).

The correlation length exponent is also determined from the susceptibility defined as

$$\chi_p = L^3(\overline{|\langle e^{2\pi i h_{\mathbf{x}}/p}\rangle|^2} - \overline{|\langle e^{2\pi i h_{\mathbf{x}}/p}\rangle|}^2). \qquad (9)$$

Near the transition point it develops a peak, whose position scales as $[\Delta^*(L) - \Delta_c] \sim L^{1/\nu}$ and whose height scales as $\chi^*(L) \sim L^{\gamma/\nu}$ with the susceptibility exponent γ. For each L, Δ^* and χ^* are obtained by fitting the susceptibility curve near the peak with a quadratic function, and then the critical exponents are extracted to yield that $\nu^{-1} = 0.76(5)$ and $\gamma/\nu = 2.90(5)$ for $p = 2$. Both estimates of ν from the magnetization and the susceptibility are consistent with each other, and the susceptibility exponent satisfies the scaling relation, $\gamma/\nu = d - 2\beta_{2,2}/\nu$ within the error bars. Figure 2(b) shows the scaling plot of $\chi_2 L^{\gamma/\nu}$ versus $(\Delta - \Delta_c)L^{1/\nu}$ with $\Delta_c = 2.20$, $\nu = 1.25$, and $\gamma/\nu = 2.90$. Except for the smallest system size $L = 4$, those exponents collapse the data well.

We have performed the same analysis for $p = 3$ and $p = 4$ and present the critical points and the critical exponents in Table I. Figures 2(c) and 2(d) show the corresponding scaling plots of $m_{p=3,q=3}$ and $m_{p=4,q=4}$. The order parameter exponent β turns out to be very small for all values of p and q. Nevertheless the transition is *not* first order since the correlation length clearly diverges at the critical point. This behavior is very reminiscent of the 3D random field Ising model (RFIM) [7,19,20] for which $\beta/\nu = 0.012(4)$ [7].

TABLE I. Estimates for the critical exponents for different commensurability parameter p obtained via finite size scaling from the numerical data.

	Δ_c	$\beta_{p,2}/\nu$	$\beta_{p,3}/\nu$	$\beta_{p,4}/\nu$	ν
$p = 2$	2.20(3)	0.046(5)	0.034(3)	0.022(3)	1.25(5)
$p = 3$	2.475(25)	0.049(7)	0.037(9)	0.024(4)	1.29(5)
$p = 4$	2.95(5)	0.044(5)	0.033(5)	0.022(5)	1.28(8)

Our numerical results deviate from the FRG results [4] in many respects. The critical exponents are substantially different from the analytic results of $\nu \simeq 2.59$ and $\beta_{2,2}/\nu \simeq 0.548$ for $p = 2$ [see Eq. (3)]. Moreover, the correlation length and the order parameter exponents appear to be independent of p within the error bars [21].

This discrepancy between the FRG and our results is surprising since *in the elastic glass phase* they agree very well. According to FRG calculations [11] the prefactor A of the logarithmic growth of fluctuations is here given by $A = \frac{\pi^2}{9}(4 - d)$. We obtain a numerical estimate for A by studying the roughness $W^2 \equiv (2\pi/p)^2[\overline{\langle h_{\mathbf{x}}^2\rangle} - \overline{\langle h_{\mathbf{x}}\rangle^2}] = \frac{1}{2L^3}\sum_{\mathbf{x}} G(\mathbf{x}) \simeq A \ln L$. Figure 3(a) shows the logarithmic scaling of the roughness W^2 in the glass phase ($\Delta > \Delta_c$), and Fig. 3(b) shows $[W^2(2L) - W^2(L)]/\ln 2$ as a function of $1/L$, which should extrapolate to A for $L \to \infty$. For $p = 3$ we get $0.98 \lesssim A \lesssim 1.11$ ($0.98 \lesssim A \lesssim 1.03$ for $p = 4$), which is also consistent with the earlier numerical work [12] on a lattice version of an elastic glass model without periodic potential [i.e., Hamiltonian (5) with $\eta_{\mathbf{x}} = 0$]. With the current system sizes finite size effects are so strong that it is not conclusive whether A is nonuniversal depending on Δ and/or p.

If the fluctuations of the elastic glass phase have the Gaussian nature as assumed in Ref. [11], the roughness, $W^2 \sim A \ln L$, and the magnetizations, $m_{p,q} \sim L^{-\theta_{p,q}}$, are not independent quantities since they should obey $\overline{\langle e^{i\phi(\mathbf{r})-i\phi(\mathbf{r}')}\rangle} \sim e^{-\frac{1}{2}\overline{\langle[\phi(\mathbf{r})-\phi(\mathbf{r}')]^2\rangle}}$ implying the relation

$$A = 2\theta_{p,p}, \qquad \theta_{p,q}/\theta_{p,q'} = q'^2/q^2. \qquad (10)$$

Figure 3(c) shows the effective exponents $\theta_{3,3}$. The polynomial fitting is used to extrapolate the asymptotic

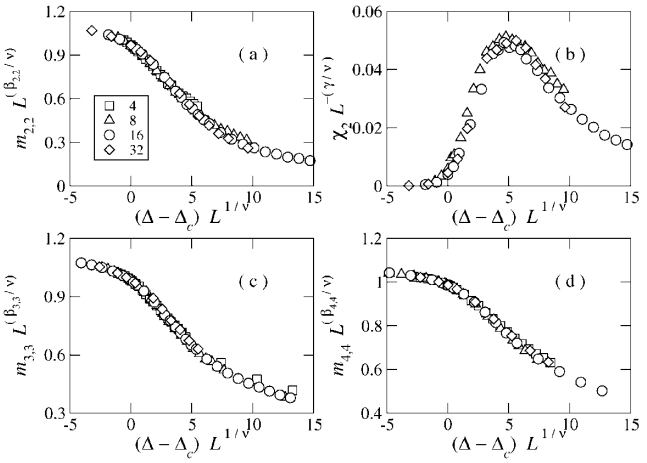

FIG. 2. Scaling plots of the magnetization for $p = 2$ (a), $p = 3$ (c), $p = 4$ (d), and the susceptibility for $p = 2$ with $\gamma/\nu = 2.90$ (b). Parameters in Table I are used in the plots.

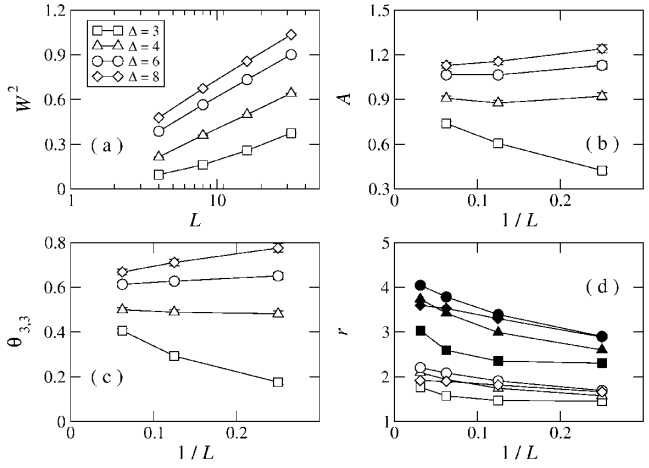

FIG. 3. (a) W^2 vs L in semilog scale, (b) prefactor A of $W^2 \sim A \ln L$, (c) effective exponent $\theta_{3,3}$ for $m_{3,3} \sim L^{-\theta_{3,3}}$, and (d) exponent ratios $r = \theta_{3,2}/\theta_{3,3}$ (empty symbols) and $\theta_{3,2}/\theta_{3,4}$ (filled symbols). All data are made from $p = 3$ in the disordered phase.

value, which yields $0.51 \lesssim \theta_{3,3} \lesssim 0.62$. We also calculate $\ln m_{3,2}/\ln m_{3,3}$ and $\ln m_{3,2}/\ln m_{3,4}$, which approach 2.25 and 4.0, respectively, as L increases; cf. Fig. 3(d). Those values satisfy the scaling relations in Eq. (10) approximately. This is strong evidence for the Gaussian nature of the fluctuations in the elastic glass phase and hence justifies the analytic approaches in this regime.

However, *at the critical point* we obtain $A_c \simeq 0.18$ ($p = 2$), 0.092 ($p = 3$), and 0.046 ($p = 4$), using again for the roughness $W_c^2 \simeq A_c \ln L$ and an extrapolation $L \to \infty$. Note that A_c appears to be approximately inversely proportional to p^2, which implies that the bare width $W_0^2 \equiv \overline{\langle h_{\mathbf{x}}^2 \rangle - \langle h_{\mathbf{x}} \rangle^2}$ is independent of p. The Gaussian theory requires the scaling relations (10) with $\theta_{p,q} = \beta_{p,q}/\nu$. But A_c and $(\beta_{p,p}/\nu)$ listed in Table I violate the first relation by a factor of 2. The ratios $\beta_{p,2}/\beta_{p,3} \simeq 1.5$ and $\beta_{p,2}/\beta_{p,4} \simeq 2.3$ are also far from the values $9/4$ and 4, required by (10). This implies a strongly non-Gaussian nature of the fixed point of the roughening transition in 3D and provides a hint why the FRG prediction (3) for 3D differs from ours. On the other hand, the latter are based on a double expansion around $d = 4$ and $p = p_c$, and it is very possible that $d = 3$ and the values for p we have considered here are simply beyond the validity of such first order perturbation expansion. We stress that we think that the system sizes we studied are sufficiently large to see the true asymptotic behavior of the roughening transition since we capture correctly the features of the rough phase fixed point.

In summary, we presented the first numerical study of a disorder-driven roughening transition in a periodic elastic medium. Our results for the critical exponents deviate significantly from the predictions of a recent analytical FRG calculation and show that the Gaussian approximation is not valid at the critical point. We found that this new universality class is reminiscent of random field critical behavior in 3D including a very small order parameter exponent. To complete the picture of the underlying zero temperature fixed point scenario, one has to compute the violation of hyperscaling exponent θ, which necessitates techniques different from those used in this work [22].

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[1] G. Grüner, Rev. Mod. Phys. **60**, 1129 (1988).
[2] G. Blatter *et al.,* Rev. Mod. Phys. **66**, 1125 (1994).
[3] G. Grüner, Rev. Mod. Phys. **66**, 1 (1994); G. Grüner, *Density Waves in Solids* (Addison-Wesley, Reading, MA, 1994).
[4] T. Emig and T. Nattermann, Phys. Rev. Lett. **79**, 5090 (1997); Eur. Phys. J. B **8**, 525 (1999).
[5] J. Villain, J. Phys. (Paris) **46**, 1843 (1985).
[6] M. J. Alava *et al.,* in *Phase Transitions and Critical Phenomena,* edited by C. Domb and J. L. Lebowitz (Academic Press, Cambridge, 2000), Vol. 18, p. 141–317.
[7] See, e.g., A. A. Middleton and D. S. Fisher, cond-mat/0107489.
[8] C. Zeng *et al.,* Phys. Rev. Lett. **82**, 1935 (1999); F. O. Pfeiffer and H. Rieger, J. Phys. A **33**, 2489 (2000); A. A. Middleton, Phys. Rev. B **61**, 14 787 (2000).
[9] J. Kierfeld *et al.,* Phys. Rev. B **55**, 626 (1997); M. J. P. Gingras and D. A. Huse, Phys. Rev. B **53**, 15 193 (1996); D. S. Fisher, Phys. Rev. Lett. **78**, 1964 (1997).
[10] S. E. Korshunov, Phys. Rev. B **48**, 3969 (1993).
[11] T. Giamarchi and P. Le Doussal, Phys. Rev. Lett. **72**, 1530 (1994).
[12] D. McNamara *et al.,* Phys. Rev. B **60**, 10 062 (1999).
[13] A. Larkin, Sov. Phys. JETP **31**, 784 (1970).
[14] Y. Imry and S. K. Ma, Phys. Rev. Lett. **35**, 1399 (1975).
[15] A related magnetic Hamiltonian with random fields was studied in A. Aharony and E. Pytte, Phys. Rev. B **27**, 5872 (1983).
[16] J.-P. Bouchaud and A. Georges, Phys. Rev. Lett. **68**, 3908 (1992).
[17] A similar model in 2D does *not* have a roughening transition: E. Seppälä, M. Alava, and P. Duxbury, Phys. Rev. E **62**, 3230 (2000); **63**, 036126 (2001).
[18] We studied also other distributions for J which give identical results. Different distributions for η and/or ϕ will be studied in [22], since in the RFIM case ($p = 2$, $J = \text{const}$) indications of nonuniversality have been reported [19].
[19] A. K. Hartmann and U. Nowak, Eur. Phys. J. B **7**, 105 (1999).
[20] A. T. Ogielski, Phys. Rev. Lett. **57**, 1251 (1986); H. Rieger and A. P. Young, J. Phys. A **26**, 5279 (1993); H. Rieger, Phys. Rev. B **52**, 6659 (1995); M. R. Swift *et al.,* Europhys. Lett. **38**, 273 (1997).
[21] Note that in [4] $\beta_{p,p}$ is the order parameter exponent, which is also p dependent in our results.
[22] J. D. Noh and H. Rieger (to be published).