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

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We study a lattice model of a three-dimensional periodic elastic medium at zero temperature with exact combinatorial optimization methods. A competition between pinning of the elastic medium, representing magnetic flux lines in the mixed phase of a superconductor or charge density waves in a crystal, by randomly distributed impurities and a periodic lattice potential gives rise to a continuous phase transition from a flat phase to a rough phase. We determine the critical exponents of this roughening transition via finite size scaling obtaining \( \nu \approx 1.3, \beta \approx 0.05, \gamma/\nu \approx 2.9 \) and find that they 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.

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 [3], where the formation of a periodically modulated structure in three space dimensions (3d) is characterized by diverging fluctuations at the transition should be dominated by a zero temperature fixed point analogous to random field critical behavior [3]. 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 [3,4], which is the method that we will 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 \( \frac{\beta}{2} (\nabla \phi)^2 \) 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 \( V_{\text{per}}(\phi) = V_{\text{per}}(\phi + 2\pi/p) \) 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]:

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

where \( \varphi(\mathbf{r}) \) are independent quenched random variables uniformly distributed on \([ -\pi, \pi ]\) and \( \gamma, \nu, \) 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 [3], but in 3d the elastic medium is stable for weak disorder [3].

For \( \nu = 0 \), the Gaussian variational and the functional renormalization group (FRG) calculations [3,11] and numerical studies [13] 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.
at large distances with a universal coefficient $A$. The overbar denotes the disorder average and $\langle \ldots \rangle$ the spatial average over $r_0$ and the thermal average.

A simple scaling argument shows that for $d > 2$ the flat phase ($\phi = 2\pi n/p$, with $n$ a fixed integer) is stable as long as the disorder is weak enough: For vanishing disorder $\eta = 0$ an excitation $\phi \rightarrow \phi + 2\pi/p$ over a terrace of linear scale $\xi$ costs an elastic energy of the order of $\xi^{d-1}$, whereas for non-vanishing 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 studied within a variational theory in [16], where a first order transition was found, whereas the FRG method used in [15] predicted a continuous roughening transition for $\mu \equiv (\pi^2/18)\epsilon > c - 4d$ at finite disorder strength that is determined by a zero-temperature fixed point. The order parameter exponent $\beta$ and the correlation length exponent $\nu$ were given to leading order in a double expansion in $\epsilon$ and $\mu = \rho^2/p^2 - 1$ by

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

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

We consider a discrete model for the continuum Hamiltonian $H$. Due to the periodic potential the elastic energy loss is calculated using a max-flow algorithm. We present numerical results obtained by using the uniform distribution for $0 \leq \phi < 2\pi$ and the exponential distribution, $P(J) = J_0^{-1} e^{-J/J_0}$, for $J > 0$. The results we report do not depend on the choice of the distribution. The strength of the random pinning potential is denoted by $\Delta \equiv V/J_0$ and we will vary this quantity to trigger the roughening transition in our system.

For each $p$, we measure the magnetizations

$$m_{p,q}(L, \Delta) = \langle e^{2m\eta_x/q} \rangle \quad (q = 2, 3, \ldots) \quad (6)$$

with $\langle \cdot \rangle$ and $\langle \cdots \rangle$ denoting the spatial and the disorder average, respectively, in the ground state. Typically the disorder average is taken over 10000 ~ 3000 samples for $L = 4 ~ 32$. Note that the order parameter $m = \langle e^{i\phi} \rangle$ considered in Ref. [15] corresponds to $m_{p,q=p}$, cf., Eq. (3).

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

$$G(r) = \langle |\phi(r_0 + r) - \phi(r_0)|^2 \rangle \simeq 2A \ln |r| \quad (2)$$

The inset shows the effective exponents for $m_{2,2}$ (Eq. (6)).

![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. (6)).](image-url)
Table I. Estimates for the critical exponents for different commensurability parameter $p$ obtained via finite size scaling from the numerical data.

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

$m_{p,q} \sim L^{-\beta_{p,q}/\nu}$, with $\beta_{p,q}$ and $\nu$ 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 $\Delta = 2.23 \pm 0.17$ when plotting $\ln m_{p,q}$ vs. $\ln L$. The critical point $\Delta_c$ can be directly determined by looking at the effective exponent

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

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 $L/\xi$ with the correlation length $\xi \sim |\Delta - \Delta_c|^{-\nu}$ such that the scaling form of the magnetization is

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

with a scaling function $F$. Using the values of $\Delta_c$ and $\beta_{2,2}/\nu$ estimated previously, we determine the correlation length exponent as the optimal value which yields the best data collapse of $m_{2,0}=2(L,\Delta)$. The estimated correlation length exponent is also listed in Table I and the scaling plot is given in Fig. 3 (a).

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

$$\chi_p = L^3 \left(\frac{\langle |e^{2\pi i h x}|^2 \rangle}{\langle |e^{2\pi i h x}|^2 \rangle^2} \right).$$

Near the transition point it develops a peak, whose position scales as $\Delta^*(L) - \Delta_c \sim L^1/\nu$ and whose height as $\chi^*(L) \sim L^{\gamma/\nu}$ with the susceptibility exponent $\gamma$. For each $L$, $\Delta^*$ and $\chi^*$ 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 $\nu$ 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. Fig. 2 (b) shows the scaling plot of $\chi^* L^{\gamma/\nu}$ 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. Fig. 2 (c) and (d) show the corresponding scaling plots of $m_{p=3,q=3}$ and $m_{p=4,q=4}$.

The order parameter exponents are so small that they might also be interpreted as a signature of a first order transition with $\beta = 0$. However, they deviate from zero systematically for all $p$ and $q$ and, furthermore, the scaling analyses show that the transition is associated with the diverging correlation length. Therefore we conclude that the transitions are of second order with small but finite order parameter exponents, which is reminiscent of the critical behavior of the 3d random-field Ising model (RFIM) [1, 5], for which $\beta/\nu = 0.012(4)$.

Our numerical results deviate from the FRG results 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 order parameter and the correlation length exponents appear to be independent of $p$ within the error bars.

The discrepancy between FRG and the numerical results is surprising since the FRG method produces the correct scaling of the elastic glass phase, i.e., the logarithmic growth of fluctuations as in Eq. (2). Then the roughness $W^2 \equiv \langle (2\pi/\nu)^2 \rangle = 1/L \sum G(0)$ also grows logarithmically in $L$ as $W^2 \simeq A \ln L$ with $A = \pi^2/6 \left(4 - d \right)$ [1]. These results are confirmed numerically for a SOS model in 3d [2], where $W^2 \simeq A \ln L$ is found with a prefactor $A \simeq 1.0$ in accordance with the analytic prediction. We also find this agreement for our model in the glass phase ($\Delta > \Delta_c$): Fig. 3 (a) shows the logarithmic scaling of the roughness $W^2$. The prefactor $A$ is estimated as $W^2(2L) - W^2(L)/\ln 2$ and plotted in Fig. 3 (b). The estimates have a strong $L$-dependence. Due to lack of a theory for corrections to scaling, we fit them with a quadratic polynomial in $1/L$ to extrapolate the asymptotic value of $A$. The results are $0.98 \lesssim A \lesssim 1.11$, consistent with the analytical and the numerical results. If the fluctuations of the elastic glass
phase have the Gaussian nature as assumed in Ref. [1], the roughness, $W^2 \sim A \ln L$, and the magnetizations, $m_{3,4} \sim L^{-\theta_{3,4}}$, are not independent quantities since they should obey \( e^{\phi(x) - \phi(y)} \sim e^{-\frac{1}{2}(\phi(x) - \phi(y))^2} \), implying the relation
\[
A = 2 \beta_{p,p} \quad \theta_{p,q}/\theta_{p,q'} = q^2/q^2. \tag{10}
\]

Fig. 3 (c) shows the effective exponents $\theta_{3,3}$. The polynomial fitting is used to extrapolate the asymptotic 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. (11) approximately. This is a strong evidence for the Gaussian nature of the fluctuations in the elastic glass phase and hence justifies the analytic approaches in this regime.

However, when using the same procedure as in the glass phase to determine $A_c$ at the critical point for $p = 2, 3, 4$, we obtain $A_c \approx 0.18$ ($p = 2$), $0.092$ ($p = 3$), and $0.046$ ($p = 4$). Note that $A_c$ appears to be approximately inversely proportional to $p^2$, which implies that the bare width $W^2_0 \equiv \langle h_x^2 \rangle - \langle h_x \rangle^2$ is independent of $p$. The Gaussian theory requires that
\[
A_c = 2(\beta_{p,p}/\nu) \quad \beta_{p,q}/\beta_{p,q'} = q^2/q^2. \tag{11}
\]
but $A_c$ and $(\beta_{p,p}/\nu)$ listed in Table I violate the first relation by a factor of two. The ratios $\beta_{p,2}/\beta_{p,3} \approx 1.5$ and $\beta_{p,2}/\beta_{p,4} \approx 2.3$ are also far from the values $9/4$ and 4, required by (11). This implies a strongly non-Gaussian nature of the fixed point 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 well 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 want to 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 we discussed the validity of its underlying Gaussian approximation. 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 $\theta$, which necessitates techniques different from those used in this work [3].

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