Critical Behavior of Pinned Charge-Density Waves below the Threshold for Sliding

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Numerical results on the static critical behavior of a collective-pinning model of charge-density waves are presented. Distinct critical behaviors are found for irreversible (typical) and reversible approaches to the threshold for sliding. From the size dependence of the threshold fields and polarizabilities, at least two distinct finite-size-scaling correlation-length exponents are identified. New analytic results on the general behavior of this model both above and below threshold are reported, including the uniqueness of the sliding state.

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Much of the electrical transport properties of materials with incommensurate charge-density waves (CDW's) can be understood in terms of the dynamics of a classical elastic CDW that is weakly pinned by impurities.[1] At low electric fields, the CDW deforms, but does not flow, and exhibits hysteretic phenomena associated with its many metastable states.[2] Above a rather sharp threshold field, the CDW moves with an average velocity, thus contributing to the transport current.[1,3] Although much of the observed behavior is qualitatively consistent with that found in numerical[4] and mean-field analyses[5] of a simple model, quantitative comparisons between theory and experiment have only just begun to be possible. This is especially true near the depinning transition, where the nonlinear interactions between many degrees of freedom give rise to novel dynamic critical phenomena.[5]

Recently, measurements[6] of the nonlinear current $j_{\rm CDW}$ for fields F just above the threshold field F_T have been fitted by the form $j_{\rm CDW} \sim (F-F_T)^{\zeta}$, with an exponent ζ which agrees *quantitatively* with numerical results[7] obtained from the simple model of a three-dimensional CDW. Experiments[8] and numerical results[4] also suggest nontrivial critical behavior *below* threshold, although definitive results are lacking. Indeed, even the *form* of the critical behavior is not understood in general, especially below threshold.

In this paper, we investigate numerically the critical behavior of the model system as the threshold field is approached from below, primarily focusing on the behavior in two dimensions, which we expect to be qualitatively similar to that in three dimensions.

The simple model[1,5] concentrates on the values of the phases $\{\varphi_i\}$ of the CDW at impurities i which lie on a d-dimensional lattice and favor particular random values $\{\beta_i\}$ of the phases. The energy of a CDW configuration is

$$\mathcal{H} = \tfrac{1}{2}\sum_{(i,j)}(\varphi_j-\varphi_i)^2 - \sum_i h_i\cos(\varphi_i-\beta_i) - F\sum_i \varphi_i\,, \qquad (1)$$

where the first term represents the elastic interaction between neighboring sites, the second term represents the periodic pinning potential, with strength $\{h_i\}$, and F represents the external electric field. The dynamics are relaxational, with equations of motion $d\varphi_i/dt = -\partial\mathcal{H}/\partial\varphi_i$.

This model exhibits two phases: a pinned static phase, with the system relaxed to a locally stable state, and a sliding phase, where the system has a nonzero average velocity v. The depinning transition between these phases occurs at a threshold field, F_T^+ for positive fields or F_T^- for negative fields, with the pinned phase existing only for $F_T^- \le F \le F_T^+$ (note that $F_T^+ \neq -F_T^-$ for a particular finite realization of the system because the impurity potential breaks the $\phi \to -\phi$ symmetry). It can be shown[9] that if the drive field is constant and is outside the static range, the system approaches a *unique, periodic, steady state,* with the system translating by 2π with the "washboard" period $T=2\pi/|v|$, a result that previously was only known empirically.[4,5]

In contrast, the behavior of this model when the field is below threshold is highly dependent on history, due to the many locally stable static configurations that exist.[1,5] An important feature of these pinned states gives rise to hysteresis: A change in the field causes local minima of the energy to vanish, so that regions of the size of the Lee-Rice length,[1] which is the scale where pinning and elastic forces are comparable, jump to nearby minima. If the field is returned to its initial value, the system will usually *not* return to its original configuration.

We find that as the field is *increased towards* threshold from a typical initial configuration, the polarization P (the mean of the phases) diverges via a series of irreversible small jumps, with an exponent $\gamma-1\approx 0.6$ in two dimensions. By contrast, if the field is *decreased from* threshold, there are no jumps and the polarization has only a weak cusp singularity which is reversible. With both of these histories, the *linear* polarizability χ (which does not include the effects of the jumps) exhibits a cusp singularity near threshold characterized by an apparently history-independent exponent $\gamma_l \approx -0.4$ in two dimensions. We study the characteristic length scales involved in these critical phenomena by investigating the finite-size scaling of various quantities. The width of the distribution of the threshold fields in finite systems and the nonlinear irreversible behavior are both characterized by correlation lengths which appear to diverge with the same exponent $\nu \approx 1$ in two dimensions. Surprisingly, the linear reversible behavior appears to be characterized by a much shorter length with exponent $\nu_l \approx 0.4$ in two dimensions. A tentative interpretation of this puzzling behavior is given in terms of the role of local modes and the "memory" of the unique threshold configuration as the field is lowered.

For our numerical simulations, we have used periodic boundary conditions on a lattice of linear size L and a fixed pinning strength $h_i = h$, with $h=5$ in two dimensions and $h=2.5$ in one-dimensional systems, chosen so that the Lee-Rice length is approximately one lattice constant. The computations were carried out on a multiprocessor Connection Machine.

Before proceeding with the numerical results, it is useful to note that there exists a "no-passing" rule for the dynamics. Consider two solutions to the equation of motion, $\{\varphi_i^1(t)\}$ and $\{\varphi_i^2(t)\}$, that are driven by two fields $F^1(t)$ and $F^2(t)$, respectively, with $F^1(t) \leq F^2(t)$, for all t. Using the convexity of the elastic potential, it can be shown[9] that if $\varphi_i^1(t) \leq \varphi_i^2(t)$ for all i at time $t=0$, then this inequality holds for all $t>0$. One immediate consequence of this rule is that the average velocity is a *unique* function of the applied field. Another is that the threshold field is *independent of history,* and the stationary configuration at threshold is *unique* modulo overall phase shifts of 2π.

We now analyze the behavior of the polarization as F_T^+ is approached. We define the reduced field $f \equiv F - F_T^+(\{\beta_i\})$ relative to the threshold field of a *particular realization* of the random system. The polarization $P(f) = L^{-d}\sum_i [\varphi_i(f) - \varphi_i^{\text{init}}]$ is measured from an initial reference configuration $\{\varphi_i^{\text{init}}\}$.

For definiteness, we chose the initial configuration to be the unique threshold configuration that is static at F_T^-, although we find qualitatively similar behavior for generic initial conditions. We then increase F adiabatically and monotonically towards F_T^+. For two-dimensional systems, we find that the polarizability for *increasing* field, $\chi^\uparrow(F) \equiv (dP/dF)^\uparrow$, is fitted well by the form $\chi^\uparrow \sim (-f)^{-\gamma}$, over roughly two decades in f for the largest system studied, with $\gamma = 1.58 \pm 0.12$ (we quote 1σ statistical error bars). In Fig. 1, we plot the shifted polarization $P - P_0$ as a function of reduced field f, for various system sizes, where the constant P_0 has been chosen to give the best fit with the form $P - P_0 \sim |f|^{-\gamma+1}$ for $|f| > 0.01$. The changes in the configuration as the field is increased consist of a smooth background and of local jumps of some of the phases that are due to local minima disappearing as F is increased. Thus, $\chi^\downarrow(F) \neq \chi^\uparrow(F)$ in general. In an infinite system the jumps occur at a dense set of fields, yielding a *smooth* $P(F)$ as F is increased.

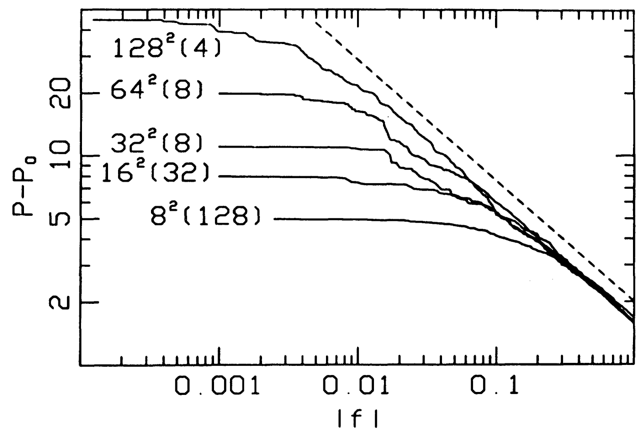

FIG. 1. Average shifted polarization $P - P_0$ vs reduced field for the irreversible approach to threshold, where $P_0 = -0.93$ has been chosen to give the best power-law fit. Data for two-dimensional systems of various sizes are shown; the number in parentheses is the number of realizations that were averaged over. The dashed line corresponds to a power law with exponent $-\gamma+1 = -0.58$ for comparison.

Even for such an irreversible path, however, it is also possible to define a *linear* differential polarizability $\chi \equiv \chi(\omega \to 0)$, which does *not* include the contribution from the jumps. Although in a finite system χ will diverge at each jump, we find that for $F < F_T^+$ in the limit of a large system $\chi(F, L, \{\beta_i\})$ converges with probability 1 to a unique value $\chi(F)$ which is a *smooth* function of F. The results for a system of size 256^2 is plotted in Fig. 2. The linear polarizability of an infinite system approaches a *finite* value, χ_T, at threshold and can be fitted with an upward cusp of the form $\chi_T - \langle \chi(f) \rangle \sim f^{-\gamma_l}$, with the exponent $\gamma_l = -0.40 \pm 0.12$ (the angular brackets denote averaging over realizations of the system). Note that this is in sharp contrast to any *finite* system, for which χ diverges at threshold with an exponent $\gamma = \frac{1}{2}$.

In contrast with the generic irreversible behavior, we find that the system can instead follow a *reversible* path over a range of field below threshold, if the initial configuration is chosen to be the one that is stationary at $F = F_T^+$. We find that the configuration follows a unique path as a function of field for F increasing or decreasing: Over a finite range of fields, *no phase jumps.* For large systems in two dimensions, $F_T = 1.49 \pm 0.01$ and the reversible range has width 0.80 ± 0.03. Such a regime of reversible behavior had been found in mean-field theory for a distribution of pinning strengths with a lower bound,[5] but perhaps it is somewhat surprising that this behavior exists in a finite-dimensional system.[10]

In the reversible regime, the differential polarizability is uniquely defined, i.e., $\chi^\uparrow = \chi^\downarrow = \chi$. We find that in two dimensions, $\chi_T - \langle \chi(f) \rangle \sim |f|^{-\gamma_l^R}$ over two decades in $|f|$

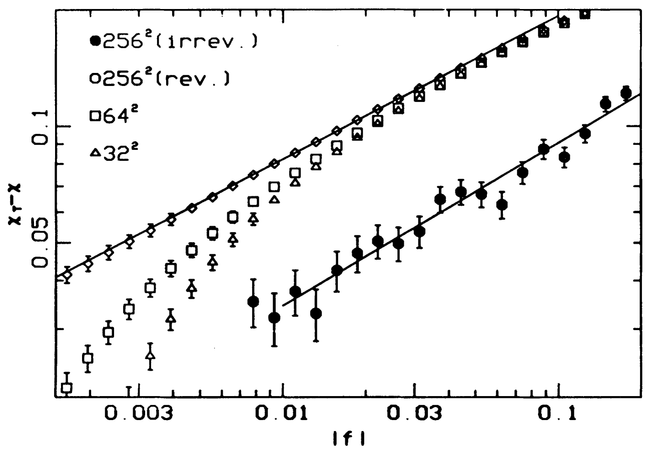

FIG. 2. *Linear* polarizability χ vs reduced field f for various system sizes in two dimensions and two different approaches to threshold. The solid symbols show the behavior for the irreversible approach for a 256^2 system, while the open symbols show the behavior in the reversible region as the field is decreased from threshold. The lines show fits by the infinite-system form $\chi = \chi_T - C|f|^{-\gamma_l}$, with χ_T the polarizability of an infinite system at threshold.

for a 256^2 system, with $\gamma_l^R = -0.37 \pm 0.05$. We have assumed that χ_T is independent of the approach to threshold—as suggested by the data.[11] Note that, within our error estimates, $\gamma_l^I = \gamma_l^R$ (but with different amplitudes for the singularity) in spite of the radical differences in the nonlinear behavior for the reversible and irreversible histories.

In order to investigate the linear polarizability further, it is useful to consider its decomposition into contributions from the eigenmodes, with eigenvalues λ_m, for the linear relaxation towards the stationary metastable configuration. We have calculated the smallest eigenvalues $|\lambda_0| < |\lambda_1| < \cdots$ in the *reversible regime.* The low-lying eigenmodes are found to be well localized, with the localization length approaching a *constant* as $F \nearrow F_T^+$. The smallest eigenvalues approximately behave as $|\lambda_m| \sim (f_m - f)^\mu$, where $f_0 = 0$ and the other f_m are positive, with $\mu = 0.50 \pm 0.01$. The modes thus appear to act as localized, almost independent, degrees of freedom each approaching a saddle-node bifurcation at the fields $\{F_T^+ + f_m\}$, with the expected individual-degree-of-freedom exponent $\mu = \frac{1}{2}$. Similar results have been found for related models.[4,12] Of course, once the field exceeds threshold, the lowest mode becomes unstable and the linear analysis no longer applies.

The linear polarizability can be simply related to the density of states $\rho(\lambda)$ and the mean-square polarization of the localized eigenmodes. We conjecture a scaling form (consistent with our results from the lowest modes)[12]

$$\rho(\lambda) \sim \lambda^\alpha \hat{\rho}(\lambda/|f|^\mu), \qquad (2)$$

with the scaling function $\hat{\rho}(\infty) \to$ const, yielding a power-law density of states *at* threshold and the exponent relation $\gamma_l = -\mu\alpha$. The apparent equality of the exponents γ_l for the reversible and irreversible histories suggests that the scaling form Eq. (2) will obtain with *both* histories, but with different scaling functions $\hat{\rho}$: In the reversible regime, $\hat{\rho}$ is zero for small values of its argument u while in the irreversible regime, the distribution of almost unstable modes will give rise to a linear density of states[5] and hence $\hat{\rho}^I(u) \sim u^{1-\alpha}$ for small u. In two dimensions our results imply $\alpha = 0.74 \pm 0.12$.

The characteristic lengths involved in the threshold critical phenomena can be investigated by the scaling with linear dimension L of various quantities, which we generally expect to be functions of L/ξ, with ξ an appropriate correlation length. The simplest quantity is the rms width of the distribution of threshold fields $F_T(\{\beta_i\})$, which fits $\Delta F_T(L) \sim L^{-1/\nu_T}$, yielding a finite-size-scaling length exponent $\nu_T = 1.05 \pm 0.04$ in two dimensions.

From Fig. 1, we can make an estimate of a characteristic length scale which controls how finite-size effects cause a crossover in the critical behavior of the *irreversible* path. In two dimensions, we find that this length diverges with an exponent $\nu_n = 1.0 \pm 0.2$, which is consistent with the ν_T found from $\Delta F_T(L)$.

The finite-size behavior of the linear polarizability along the *reversible* path, shown in Fig. 2 for two dimensions, can be scaled to fit[11] a single function of $L|f|^{\nu_l}$, with $\nu_l = 0.4 \pm 0.1$. This ν_l is much less than ν_n and ν_T, so that the finite-size corrections in this regime are far smaller than in a hysteretic path, suggesting a *second, distinct* correlation length. The scaling function can be understood in terms of the domination of the singular part of the linear response by a single degree of freedom as $f \to 0^-$, which contributes a term to χ of order $f^{-\mu}/L^d$. This yields the scaling relation $d\nu_l = \mu - \gamma_l^R$, which is consistent with our numerical results in two dimensions and also with mean-field theory.[9]

The various finite-size-scaling correlation-length exponents can be compared with a general bound which is essentially due to the independence of different parts of a random system. It has been proven[13] that in a random system any finite-size-scaling length that can be defined in a certain probabilistic manner (essentially in terms of the probability that a finite system behaves as if it were above threshold) will, if it diverges, do so with an exponent $\nu_f \geq 2/d$. The exponent ν_T defined from $\Delta F_T(L)$ must (up to minor technicalities) obey this bound, consistent with our numerical results in two dimensions. Preliminary data also suggest that ν_T satisfies this bound in one dimension.

Because the generic irreversible approach to threshold is triggered by a series of local thresholds of subsystems, we would expect that the approximate independence of these subsystems would yield a finite-size-correction exponent for the polarization which also satisfies the bound, $\nu_n \geq 2/d$, consistent with the numerical results. Indeed, it is reasonable to attribute these finite-size corrections to an intrinsic correlation length of the infinite system—diverging with the same exponent —which characterizes the size of the "avalanches" which occur when a local mode goes unstable. This clearly merits further investigation, and perhaps suggests a route to relating various exponents. It also suggests possible parallels with other "avalanche" phenomena found in a variety of different systems.[14]

The finite-size-scaling exponent ν_l in the reversible regime is more problematical: It clearly violates the $2/d$ bound. This unexpected feature is presumably due to the infinite-range correlations which persist due to the special preparation of the system in its threshold configuration, which is a unique state determined by the *whole* system.[15]

In summary, we have numerically investigated the critical behavior and finite-size scaling in a simple model of charge-density waves as the threshold field is approached in the pinned phase. We find two distinct approaches to threshold, characterized by some different and some similar exponents and at least two distinct lengths which diverge at threshold. The relationship between the various exponents and also the connections with the critical behavior above threshold are both subjects of continuing investigation. Webman[16] has studied a simplified model of CDW's below threshold which does not have jumps. The exponents he finds are thus likely to be for a different universality class.

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[10]Note that the nonzero width of the reversible regime may depend on the distribution of pinning strengths h_i, or the distribution of impurity positions in more realistic models.

[11]We actually used $d\chi/df$ to study the linear polarizability, since the divergence of χ at threshold in a finite system made $\chi_T(L=\infty)$ hard to calculate directly.

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[15]Note that the width of the distribution of χ must be at least $O(L^{-d/2})$ even though the finite-size effects in a typical sample occur on a scale of $f \sim L^{-\nu_l}$. The theorem of Ref. 13 does *not* apply to the latter quantity. A somewhat analogous effect occurs at a conventional first-order phase transition in the presence of random fields.

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