Critical Dynamics of a Pinned Elastic Medium in Two and Three Dimensions: A Model for Charge-Density Waves

P. Sibani[(a)] and P. B. Littlewood
AT&T Bell Laboratories, Murray Hill, New Jersey 07974
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We study numerically the dynamical equilibrium behavior for the uniformly driven, elastic model of Fukuyama, Lee, and Rice for pinned charge-density waves, in the critical region close to the threshold field for sliding, in two and three dimensions. We obtain a critical exponent for the mean velocity in good agreement with recent experiments, and scaling for the velocity correlation function, from which we extract a diverging correlation length. The correlation-length exponent ν is found to be less than $2/d$ (d is the dimension), suggesting unusual critical behavior for this model.

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The model of Fukuyama, Lee, and Rice[1] (FLR) for the dynamics of sliding charge-density waves (CDW) has been extensively studied not only for its applications to real materials,[2] but also as a paradigm for the behavior of nonlinear many-effective-degree-of-freedom systems.[3] The FLR model describes a classical, spatially extended system interacting with quenched random impurities and under the influence of a driving electric field; it is equivalent to a system of coupled, overdamped nonlinear pendula. A very similar model can be used to describe the pinning of a votex lattice by disorder in a type-II superconductor.[4] The many-degree-of-freedom nature of this model is particularly crucial in the description of the behavior close to the threshold electric field (E_T) for sliding; the depinning may be regarded as a dynamic critical phenomenon.[5] It is described by exponents which are different from one-dimensional systems such as circle maps, which are often used in modeling CDW dynamics.

Owing to the large computational effort required for short-range interactions, the *critical* behavior has previously been studied only in mean-field theory[5] with some limited numerical work in one dimension;[3] more extensive numerical studies have been performed on the 1D model with incommensurate, rather than random, pinning.[6] By utilizing parallel computational techniques on a Thinking Machines Corp. CM-2 computer, we have successfully equilibrated large systems[7] (up to 2^{18} sites) close to threshold, and can thus study the critical behavior without the usual recourse to finite-size scaling methods. The good agreement we find between the calculated velocity exponent in dimension $d=3$ and recent experimental data on $NbSe_3$ (Ref. 8) is an important *quantitative* test of the model. Our 2D results should be relevant for vortex motion in thin superconducting films, provided phase-slip processes can be neglected.

The FLR model treats the CDW charge density $\rho(\mathbf{r}) = \rho_0 \cos[\mathbf{Q}\cdot\mathbf{r}+\phi(\mathbf{r})]$ as a deformable elastic medium, with the local position of the CDW described by a phase $\phi(\mathbf{r})$, and the dynamics given by the following equation of motion:

$$\gamma\dot{\phi}(\mathbf{r}) = K\nabla^2\phi(\mathbf{r}) + \sum_i V_i \delta(\mathbf{r}-\mathbf{R}_i)\sin[\theta_i+\phi(\mathbf{r})] + E(t)\,. \tag{1}$$

Here we have assumed short-range interactions with impurities at random positions $\mathbf{R}_i$, so that $\theta_i = \mathbf{Q}\cdot\mathbf{R}_i$ is a random number, uniformly distributed in $(0,2\pi)$. For numerical simulation, we discretize the equation using a standard finite-difference method on a cubic grid, obtaining[3]

$$\phi_i(t+\delta t) = \phi_i(t) + \delta t\{K\Delta^{(2)}\phi_i(t) + V_i \sin[\theta_i+\phi_i(t)] + E(t)\}\,, \tag{2}$$

where $\Delta^{(2)}\phi_i$ is the discrete second difference between neighboring lattice points. While other more refined discretization methods are available, ours lends itself to a simple physical interpretation as a model of elastically coupled damped oscillators. For the critical behavior, the details of the discretization are not expected to be relevant.[3] In the simulations V_i was chosen randomly to be zero or a constant V, with roughly half of the lattice sites having nonzero pinning. We used values of V and K such that both the characteristic length scale $\xi_0 \approx (V/K)^{1/2}$ and the threshold field E_T are of order unity. We used periodic boundary conditions on an N^d cubic system, with $N=128$ and 256 in two dimensions, and $N=16$, 32, and 64 in three dimensions.

It is important to be able to separate the transient response from the dynamical equilibrium behavior reached at long times. For a sliding state, it is clear that each grid variable must return to its initial value modulo 2π. Let the sequence of times $t_1, t_2, \ldots, t_n$ be the recurrence times for a particular grid point, henceforth called the "central variable" and which acts as an internal clock. At each of these times we compare the global solutions with their values at the previous "tick" t_{n-1} of the clock, by computing both Euclidean and max norms. The solution is periodic when both these measures of distance become zero, and when the period $T = t_n - t_{n-1}$ becomes constant. The mean velocity $v = \langle\dot{\phi}\rangle$ is identically

$2\pi/T$. With a uniform dc applied field, we find always that the dynamical solutions above threshold are periodic in time, as inferred already in one dimension.[3] Consequently, there is no broadband noise (BBN) for uniform driving, and narrow band noise (NBN) occurs only as a finite-size effect, as found by perturbation theory to all orders in $1/E$.[9] Our method is easily adaptable to search for cycles of longer periods (by comparing the configurations at times t_n, t_{n-j}) such as occur when the driving field also has an ac component. These periodicities would also be revealed by Fourier analysis, but this is impracticable for an accurate determination of the periods, requiring very long integration times.

Close to the threshold field, we find that the mean velocity satisfies

$$v = N^{-d}\sum_i \langle \dot\phi(r_i)\rangle \sim f^{\zeta}, \tag{3}$$

where the reduced field is $f=(E-E_T)/E_T$. The cooperative nature of the behavior is made explicit by defining a correlation length $\xi \sim f^{-\nu}$ from the equal-time correlation function for the velocities:[5]

$$C(r_j) = N^{-d}\sum_i \langle \dot\phi(r_i+r_j)\dot\phi(r_i)\rangle - v^2 \sim \Delta^2(f) c(r_j/\xi(f)), \tag{4}$$

where $\Delta \sim f^{\psi}$ measures the rms velocity fluctuations and the scaling form is expected to be valid for both $r,\xi \gg \xi_0$. The angular brackets in Eq. (4) specify a time average; while strictly unnecessary for an infinite system this improves the statistics in finite-size lattices. We note that $\sum_i C(r_i)=0$, so that $C(r)$ is a function with a decaying envelope and at least one change of sign.[10] Our data are consistent with a functional form for the scaling function of

$$c(x) = x^{-\kappa} c'(x), \tag{5}$$

where c' is an oscillatory function of its argument,[11] and the power-law prefactor is expected in general.[5] The on-site correlation function $C(0)=\Delta_0^2 \sim f^{2\psi_0}$ also vanishes with a power-law exponent at threshold, which suggests that the critical regime (defined by $\Delta_0/v > 1$) should be over a field range ~ 1 in reduced field. Note that consistency of the above scaling relations requires that $\psi_0 = \psi - \frac{1}{2}\kappa\nu$, a relation obtained by matching $C(0)$ to $\Delta^2 c(\xi_0/\xi)$ at the short scale $r \sim \xi_0$.

In Fig. 1 we show the results obtained in three dimensions for single runs with $N=16$ and $N=64$ and three configurations at $N=32$. Because there is a divergent length scale ξ at threshold, finite-size effects will modify the critical behavior, leading to a crossover to $\zeta=\frac{1}{2}$ when $\xi \sim N$. The finite-size effects are clearly visible at low reduced fields for $N=16$ and less so for $N=32$, but computational times were too long for this regime to be reached for $N=64$. At higher fields than shown here, we find systematic deviations away from power-law scaling consistent with the high-field perturbation theory.[12] The critical region can also be estimated by comparing the on-site rms fluctuations of the velocity Δ_0 with the mean velocity v; we find that $\Delta_0 > v$ for $f \lesssim 3$. This, and the analysis of the correlation length ξ given below, gives us confidence that the crossovers at low and high velocities are well controlled. We fit the critical exponent for the larger sizes over a range of velocities from $10^{-2} < v < 1$, obtaining $\zeta = 1.16^{+0.04}_{-0.02}$ in three dimensions; the uncertainty in the exponent is determined principally by the accuracy in determining E_T. A recent experimental

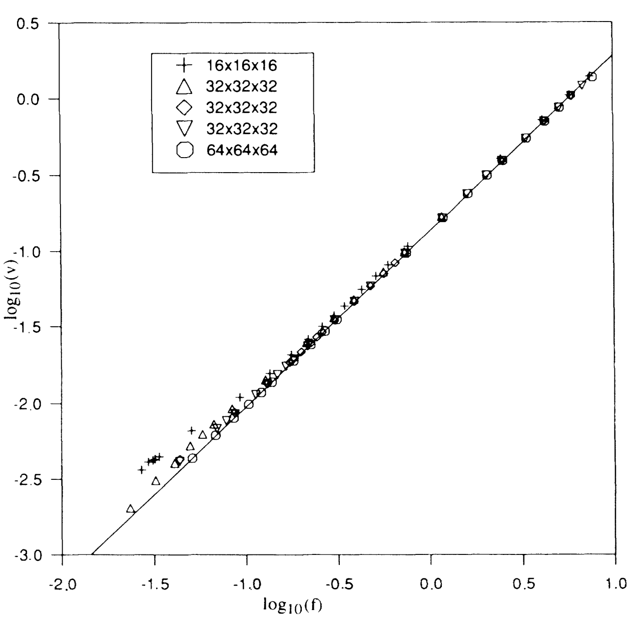

FIG. 1. Plot of the mean velocity vs the reduced field for five samples of three different sizes in three dimensions.

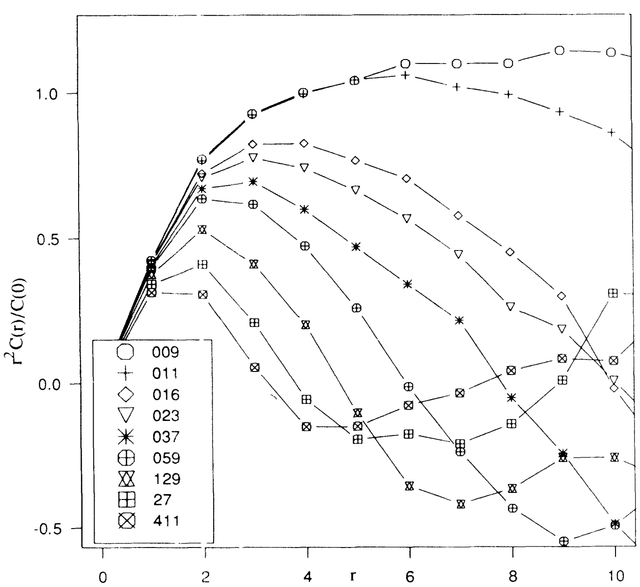

FIG. 2. Velocity-velocity correlation function $r^2C(r)/C(0)$ for a two-dimensional system of size 128^2. The symbols are labeled by the reduced field $(E-E_T)/E_T$.

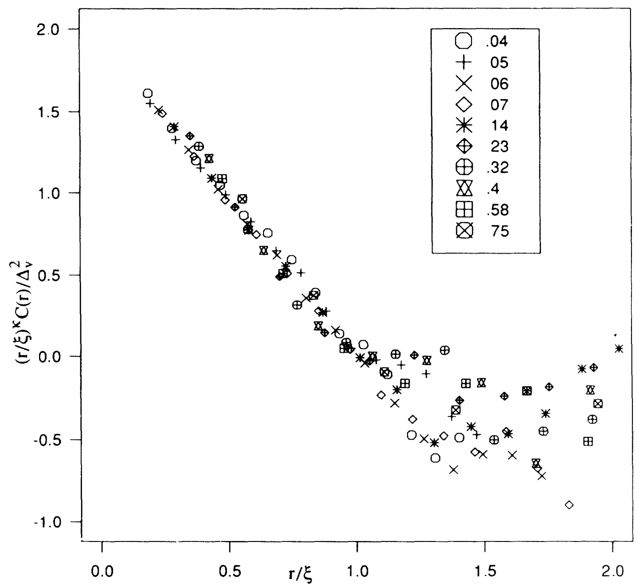

FIG. 3. Scaled correlation function $(r/\xi)^\kappa C(r)/\Delta^2$ vs the scaled distance r/ξ for a three-dimensional system of size 32^2; the fit has $\kappa = 1.8$ and the symbols are labeled by the reduced field.

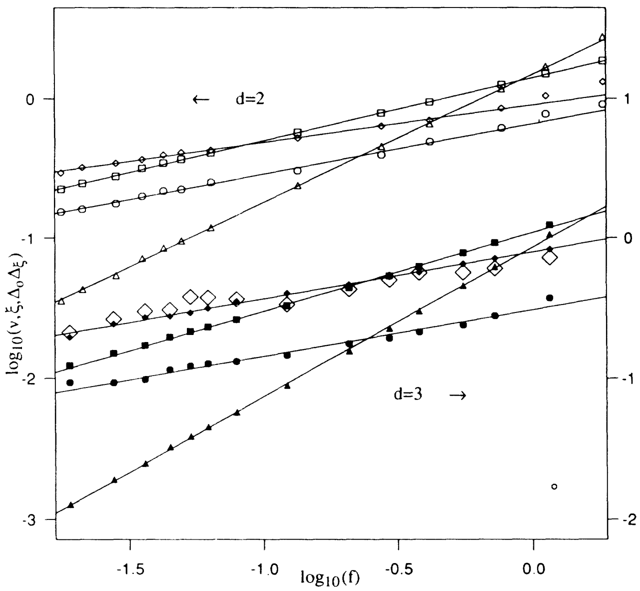

FIG. 4. Logarithmic plot vs reduced field of the correlation length ξ^{-1} (circles), mean velocity v (triangles), on-site rms velocity Δ_0 (squares), and the rms velocity Δ_ξ integrated over a correlation volume (diamonds), in two ($N = 128$, open symbols, left-hand scale) and three ($N = 32$, filled symbols, right-hand scale) dimensions. The straight lines are least-squares fits to the data, ignoring points close to E_T. The large diamonds are the NBN amplitude ($d = 3$, integrated over all harmonics) for comparison to Δ_ξ.

measurement by Bhattacharya, Higgins, and Stokes[8] on $NbSe_3$ yields a value for the exponent of 1.23 ± 0.07; as expected, both numerical and experimental results are lower than the mean-field value of $\zeta = \frac{3}{2}$.[5]

In Fig. 2, we show the calculated correlation function $r^2 C(r)/\Delta_0^2$ for a two-dimensional 128^2 system. The oscillatory character of the correlation function is clear. Even very close to threshold, the correlation function falls off rapidly with distance, indicating that the microscopic scale ξ_0 remains relevant at threshold, and that at length scales $\xi_0 \ll r \ll \xi$, the correlation function falls off as a power law. We determine a length scale $\xi(f)$ from the first zero crossing of $C(r)$, and then rescale the data to determine Δ and the scaling function $c(x)$. We find that our data are consistent with the functional form of Eq. (5).[11] This is demonstrated in Fig. 3 for a three-dimensional 32^3 system where we plot the rescaled correlation function $(r/\xi)^\kappa C(r)/\Delta^2$ against the scaled length r/ξ. At small distances $r \sim \xi_0$ no power-law distance dependence is expected of course, although by including a smooth crossover on short length scales it is possible to include the short-scale information. However, we obtain no new information at the expense of an additional fitting parameter so we have chosen not to do this here; in Fig. 3, we have suppressed the first two data points (our parameters are such that $\xi_0 < \sim 1$), and plot only data for $r \gtrsim 2$. For $r/\xi \gtrsim 1$ there is considerable scatter in the data points; in this region, the value of the correlation function is $< 10^{-2} C(0)$ and small absolute fluctuations are enhanced by the large factor $(r/\xi)^\kappa$. Since the important information in the correlation function is buried in the tail, the behavior at distances longer than the correlation length cannot be determined from the present data. However, the field dependence of the characteristic scale ξ and amplitude Δ can be obtained independent of the specific form of the scaling function.

The extracted results for ξ, Δ_0, and v are shown in Fig. 4; in addition, we plot the rms velocity fluctuations integrated numerically over a correlation volume: $\Delta_\xi = [\int_\xi d^d r\, C(r)]^{1/2} \sim f^{\psi_1}$. The values of exponents are collected in Table I, and compared with the earlier results from mean-field theory and numerical simulations in one dimension. Two of the exponents are redundant, and provide a check on our chosen scaling form; we should find (and do, within error estimates) $\psi_1 = \psi - \frac{1}{2} d\nu$ and $\psi_0 = \psi - \frac{1}{2}\kappa\nu$. The 3D data shown in Fig. 4 are from the same run as the triangles in Fig. 1; the lowest three points deviate from the power-law fit in Fig.

TABLE I. Critical exponents for the FLR model in two and three dimensions, compared with earlier results in one dimension (Ref. 3) and from mean-field theory (Ref. 5).

	$d=1$	$d=2$	$d=3$	$d=\infty$
ζ	0.85 ± 0.15	0.95 ± 0.05	1.16 ± 0.04	$\frac{3}{2}$
ν	0.2 ± 0.1	0.38 ± 0.05	0.36 ± 0.10	$\frac{1}{2}$
ψ		0.72 ± 0.04	0.95 ± 0.05	
κ		1.4 ± 0.3	1.8 ± 0.4	
ψ_0	0.3 ± 0.1	0.47 ± 0.03	0.62 ± 0.05	
ψ_1		0.28 ± 0.05	0.37 ± 0.10	

1 and also show clear evidence of finite-size effects in the correlation length ξ (Fig. 4), which gives us further confidence that the effects of finite size are under control.

We note that within very close bounds we find $\psi_0 = \frac{1}{2}\zeta$. This relation is a simple consequence of the jerky motion of the CDW close to threshold, where the local velocity is ~ 1 for short periods separated by times $\sim 1/v$ when the local velocity makes a negligible contribution to the average.[6] Thus *all* moments of the local velocity average will scale as mean velocity: $\langle [N^{-d}\sum_i \dot\phi(r_i)]^n \rangle \simeq v$. The existence of a finite length scale at E_T can also be inferred directly from the mean velocity as a function of time in the critical regime.

Although for an infinite system the mean velocity will be time independent, statistical fluctuations for finite N lead to a periodic component at the "washboard," or NBN, frequency $2\pi/T = v$. Close to threshold, we find that the measured spatially averaged velocity acquires considerable harmonic content; in a finite sample of volume V, the amplitude of the coherent NBN is expected to be given by fluctuations in the velocity of a correlated volume, and should be of order $\Delta[\xi^d/V]^{1/2} \sim f^{\psi_1}$. Since $\psi_1 < \zeta$, the NBN will dominate the dc velocity close to threshold. This offers a possibility for a further experimental check of the scaling behavior. Because our simulations have been performed only for large sizes, it was not possible to check unambiguously the square-root volume dependence, although this is well established by the perturbation theory.[9] In Fig. 4, we show the measured NBN amplitude (integrated over all harmonics) for a 32^3 sample; there are large fluctuations (as expected for a finite-size effect) but the data are consistent with f^{ψ_1}.

While there is some considerable uncertainty as to the extraction of ξ from our data, we believe that the results for ν are unambiguously *inconsistent* with the relation $\nu \geq 2/d$, believed to be a general result for quenched disorder.[13] This result was derived from contemplation of a finite-size scaling procedure, whereas we have extracted ξ directly from the correlation function. Thus it is possible that there are two (or more) diverging lengths involved in the approach to threshold, with ξ determining the growth of local velocity correlations (in particular, the spatial oscillations of the correlation function).[14] We also remark that an earlier experimental analysis of the BBN near threshold was interpreted by means of a threshold-field fluctuation model and indicated a correlation-length exponent of $\nu \approx \zeta/3$,[15] consistent with our value. However, since no BBN is found in the uniformly driven FLR model, the analysis of BBN experiments depends on assumptions as to its origin, which are difficult to check.

In conclusion, we have determined critical exponents and scaling of the correlation function for the FLR model in two and three dimensions. The velocity exponent in $d=3$ is in good agreement with experimental results, and the observation of a nontrivial exponent for the dynamics adds further to the already considerable evidence that the many-degree-of-freedom nature of CDW's is a central feature of their dynamics.

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[a]Permanent address: Department of Physics, University of Odense, Campusvej 55, 5230 Odense M, Denmark.

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