PHYSICAL REVIEW A VOLUME 36, NUMBER 12 DECEMBER 15, 1987

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Scaling anomaly at the critical transition of an incommensurate structure

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(Received 22 July 1987)

We study the critical behavior of a Frenkel-Kontorova model, extended to include a second harmonic of the external potential. For certain parameter values of the model the transition from the locked to the sliding incommensurate phase shows a scaling anomaly for the correlation length, with the critical exponent varying with the potential. We conjecture that this behavior indicates a crossover to a new universality class.

The physics of incommensurably modulated structures poses a variety of important and challenging questions.[1] One model, albeit a very crude rendering of a real incommensurate system, has played an important role in addressing these questions: this is the Frenkel-Kontorova (FK) model.[2] Here one considers a one-dimensional lattice of particles $\{x_0, \dots, x_N\}$, with a nearest-neighbor elastic interaction,

$$W(x_j,x_{j-1}) = \tfrac{1}{2}(x_j - x_{j-1} - \delta_0)^2 , \quad (1)$$

x_j being the position of the jth particle, and δ_0 a dislocation parameter. The particles are subject to an external potential V_1, usually taken to be sinusoidal,

$$V_1 = \lambda_1 \sum_j [1 - \cos(2\pi x_j/L_1)] . \quad (2)$$

The problem has two natural length scales: the average lattice spacing δ and the periodicity L_1 of the potential. Rather surprisingly, considering the simplicity of the model, the competition between the two scales generates a number of intriguing phenomena. In particular, as shown by Aubry,[3] if δ via the boundary condition

$$\delta = \lim_{N\to\infty} \frac{x_N - x_0}{N} \quad (3)$$

is chosen incommensurate with L_1 (i.e., δ/L_1 approaches an irrational number), the ground state undergoes a structural phase transition at a well-defined value $\lambda_1 = \lambda_1^c$. When $\lambda_1 < \lambda_1^c$, the lattice responds smoothly to an infinitesimal displacing force (*sliding phase*), while for $\lambda_1 > \lambda_1^c$ the particles remain locked to their positions (*pinned phase*). The pinning transition, with $\lambda_1 > \lambda_1^c$, is of second-order type, characterized by a critical exponent $\nu = 0.99$ for the correlation length.[4-7]

What happens if a third length scale is introduced into the problem, e.g., by adding a term,

$$V_2 = \lambda_2 \sum_j [1 - \cos(2\pi x_j/L_2)] , \quad (4)$$

to V_1? If L_2 is incommensurate with both δ and L_1, there are reasons to expect that the system will develop a disordered ground state.[8] On the other hand, with L_2 commensurate with L_1, the ground state is still incommensurably modulated.[9] In this latter case it is of interest to ask if, and how, the critical behavior at the pinning transition will be influenced by the presence of the new scale L_2. One can show, by topological arguments,[9] that the structure of the ground state is linked to the local structure of certain trajectories in a class of area-preserving twist maps, and thus, the problem can be attacked by a direct study of these maps. Renormalization-group arguments, as well as numerical studies of twist maps, seem to favor the existence of one (or several) universality class(es) of systems with identical scaling behavior.[4,5] In fact, as we will show below, the critical behavior is rather more intricate, characterized by a scaling anomaly in certain ranges of values for λ_1 and λ_2, with the critical exponent for the correlation length varying with the external potential.

For simplicity we study the model with $L_2 = \frac{1}{2} L_1$, and thus take for the free energy at zero temperature,

$$\mathcal{F} = \sum_j \tfrac{1}{2}(x_j - x_{j-1} - \delta_0)^2 - \frac{\lambda_1}{(2\pi)^2}[1-\cos(2\pi x_j/L_1)] - \frac{\lambda_2}{(4\pi)^2}[1-\cos(4\pi x_j/L_1)] \ , \tag{5}$$

where we have rescaled λ_1 and λ_2, defined in the range $\lambda_1 > 0$, $\lambda_2 \geq 0$.

This is a discrete version of the double sine-Gordon model, and might be of relevance for, e.g., the study of misfit dislocation on an Au(111) reconstructed surface.[10] The equilibrium equations,

$$\frac{\partial \mathcal{F}}{\partial x_j} = 0 \ , \tag{6}$$

with $L_1 = 1$ generate the area-preserving twist map,

$$p_{j+1} = p_j - \frac{\lambda_1}{2\pi}\sin(2\pi x_j) - \frac{\lambda_2}{4\pi}\sin(4\pi x_j) \ ,$$
$$x_{j+1} = x_j + p_{j+1} \ , \tag{7}$$

with $p_j \equiv x_j - x_{j-1}$. In what follows we restrict the map to the torus $[0,1] \otimes [0,1]$.

As for the standard FK model, the incommensurate ground state in the sliding phase is represented by a Kolmogorov-Arnold-Moser (KAM) trajectory, nonhomotopic to zero, with winding number $\omega = \delta$. As the parameters λ_1 and λ_2 are increased, this trajectory breaks up into a fractal object, a *cantorus*,[11,12] representing the ground state in the pinned phase. We choose $\omega = \frac{1}{2}(\sqrt{5}+1)$ *(golden mean)*, and study the corresponding KAM curve via its approximating minimax orbits[13] with winding numbers $\omega_n = F_{n+1}/F_n$.

Here $\{F_n\}$ are the Fibonacci numbers, with the sequence $\{\omega_n\}$ converging to the golden mean. The breakup of the curve is signaled by a loss of stability of the minimax orbits, as measured by the residue $R = \frac{1}{4}(2 - \mathrm{Tr}M)$, where M is the Jacobian of the map. Iterating the map and employing the residue criterion,[14] i.e., identifying the map parameters for which $R = 0.25$ in the limit of large n, the critical pairs $(\lambda_1^c, \lambda_2^c)$ can hence be determined. The resulting phase diagram is shown in Fig. 1, with the area below (above) the curve representing the sliding (pinned) phase. In Fig. 2 we exhibit two trajectories at criticality, approximated by minimax orbits with winding numbers 987/610.

It is important to stress that there is a difference between the phases for $\lambda_1 = 0$ and those for $\lambda_1 \neq 0$. Along the critical line, with $\lambda_1 \neq 0$, the local behavior of the trajectories shown in Fig. 2 can be expected to be controlled by the fixed map renormalization for the golden mean winding number, described below. On the other hand, at the endpoint, $\lambda_1 = 0$, the period of the trajectory is halved, so the winding number is doubled,[15] leading to a different renormalization.

Turning to the scaling behavior in the critical region, we focus on the correlation length ξ, defined by

$$\delta x_m \sim \exp(-|m-k|/\xi)\,\delta x_k \ . \tag{8}$$

ξ measures the distance over which a perturbation δx_k propagates along the lattice, and, as follows from its definition, is the inverse of the Liapunov exponent for the trajectory representing the ground state. To study scaling of the correlation length in the supercritical region, we approximate the golden mean cantorus with the minimizing orbits[13] with winding numbers ω_n, and compute their Liapunov exponents over some range $\lambda_j \geq \lambda_j^c$, $j = 1,2$.

We take 14 pairs $(\lambda_1^c, \lambda_2^c)$ on the critical line (see Table I), and for each pair study the map for six values of λ_1 in the supercritical region $|\lambda_1 - \lambda_1^c| \leq 0.02$, holding λ_2 fixed. The obtained results imply a power-law behavior

$$\xi_n \sim (\lambda_1 - \lambda_1^c)^{-\nu_n} \ , \tag{9}$$

where ξ_n is the inverse Liapunov exponent for the minimizing orbit with winding number ω_n. As $n \to \infty$, the orbits converge to the cantorus and $\xi_n \to \xi$ with $\nu_n \to \nu$, ν being the critical exponent for the correlation length. For

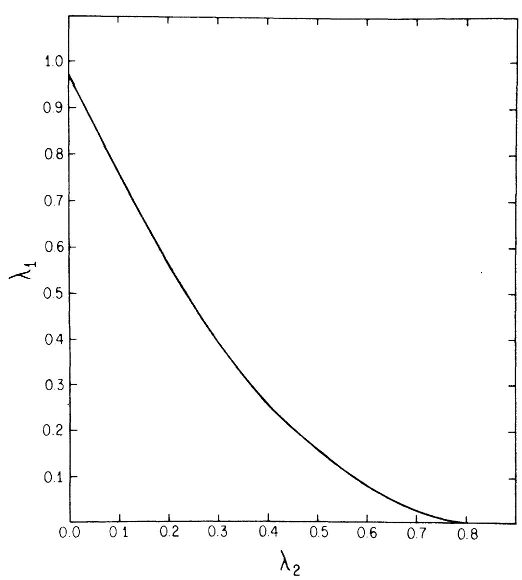

FIG. 1. Phase diagram in the (λ_1, λ_2) plane. The area below (above) the critical line represents the sliding (pinned) phase. The intersections with the λ_1 and λ_2 axes are given by $\lambda_1^c = 0.971\,64$ (critical point in the standard FK model) and $\lambda_2^c = 0.804\,72$, respectively.

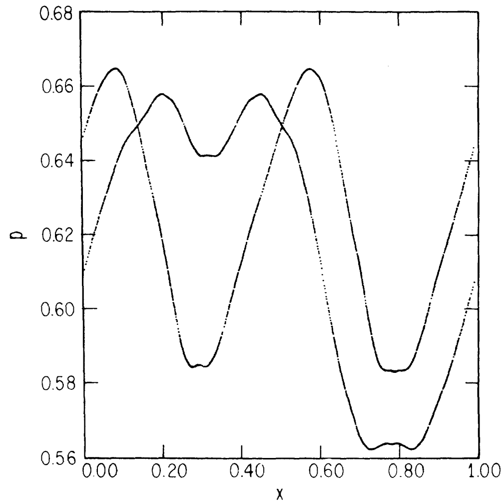

FIG. 2. Critical trajectories approximated by minimax orbits with winding number 987/610. The trajectory hitting the vertical axis at $p=0.645$ and $p=0.609$ corresponds to the critical point $(\lambda\mathfrak{f},\lambda\mathfrak{s})=(0.02441,0.70000)$ and $(0.56156,0.20000)$, respectively.

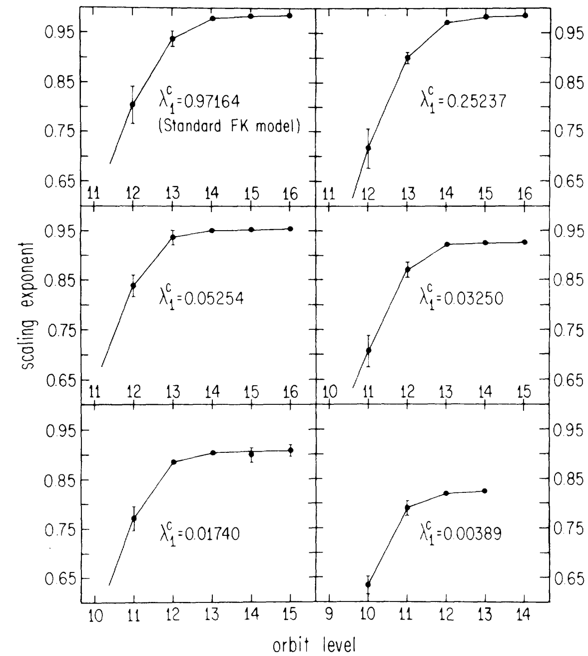

FIG. 3. Scaling exponents vs orbit levels for scaling in λ_1.

$\lambda\mathfrak{f}\geq 0.08\pm 0.02$, the value of v is consistent with the golden mean exponent:[4–7] extrapolation from level $n=16$ yields $v=0.99\pm 0.005$. As an illustration, in Fig. 3 we display two sequences for $\lambda\mathfrak{f}=0.97164$ (standard FK model), and $\lambda\mathfrak{f}=0.25237$, respectively. However, for $\lambda\mathfrak{f}\leq 0.08\pm 0.02$ the sequence of v_n do *not* converge towards the expected value 0.99. Instead the convergence is now towards exponents which decrease monotonically with $\lambda\mathfrak{f}$ (see Fig. 3). We estimate the lower bound at the endpoint $\lambda\mathfrak{f}=0$ to be $v=0.60\pm 0.02$.

This behavior may suggest the existence of a new fixed point under renormalization of the map. In fact, as we have already hinted, there is at least one additional fixed map which can be found by exploiting the renormalization operator[4,5]

$$N_1\begin{pmatrix}U\\T\end{pmatrix}\equiv B\begin{pmatrix}T\\TU\end{pmatrix}B^{-1}\,, \tag{10}$$

where T and U are a pair of commuting maps and B is a scaling operator. In the parameter range where $v=0.99$, the critical trajectory of winding number ω is locally given in terms of the well-known[4,5] fixed map N_1. On the other hand, when λ_1 goes to zero the physical winding numbers of the critical trajectory discontinuously jumps to $2\omega=\omega^3-1$. Since ω^3 has the continued fraction representation $[4,4,\ldots,4]$, the critical trajectory for $\lambda_1=0$ is given in terms of the fixed map of

$$N_4\begin{pmatrix}U\\T\end{pmatrix}\equiv B\begin{pmatrix}T\\T^4U\end{pmatrix}B^{-1}\,. \tag{11}$$

It follows from the cubic relations between the numbers ω and 2ω that the critical fixed map of Eq. (11) is directly related to a three-cycle of Eq. (10). This three-cycle is a higher-order solution of Eq. (10), analogous to the higher-order fixed points of period doubling.[16] Numerical

TABLE I. Points on the critical line in Fig. 1.

$\lambda\mathfrak{f}$	$\lambda\mathfrak{s}$	$\lambda\mathfrak{f}$	$\lambda\mathfrak{s}$
0.86836	0.05000	0.05254	0.64000
0.76441	0.10000	0.03250	0.68000
0.56156	0.20000	0.02441	0.70000
0.38538	0.30000	0.01740	0.72000
0.25237	0.40000	0.00599	0.76000
0.15458	0.50000	0.00389	0.77000
0.07757	0.60000	0.00225	0.78000

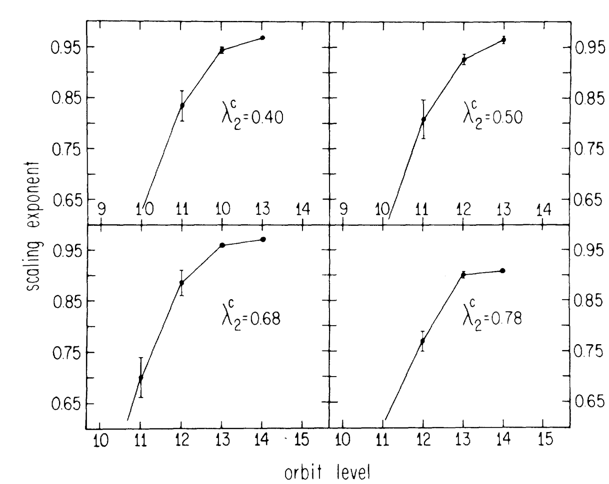

FIG. 4. Scaling exponent vs orbit levels for scaling in λ_2.

observations of the linearization of Eq. (11) around the fixed map of Eq. (11) show that there is one relevant eigenvalue, of magnitude very close to $\omega^3=4.23$. Similarly, linearizations of Eq. (10) around the three-cycle of Eq. (10), show, as it must, that 4.23 is a relevant eigenvalue. In addition, since perturbation of the three-cycle solution of Eq. (11) can diverge in the direction of the well-known critical fixed map of that equation, there must be a second relevant eigenvalue in this case. Unfortunately, we have been unable to estimate it.

Analagous to examples in finite-temperature critical phenomena,[17] our results suggest that the apparent "nonuniversal" scaling observed numerically is a manifestation of a crossover to the doubled winding-number fixed point. We wish to emphasize, however, that we have as yet no independent observations to support this hypothesis.

The picture takes on an added twist when studying scaling in λ_2 for nonzero λ_1^c. Choosing the same critical points as above and repeating the analysis, now keeping λ_1 fixed, we find

$$\xi_n \sim (\lambda_2-\lambda_2^c)^{-\nu_n} . \tag{12}$$

Some of the sequences $\{\nu_n\}$ are displayed in Fig. 4. The instabilities of the supercritical orbits are now more severe, which prevents us from reaching a level where the convergence is evident. Nevertheless, the obtained results again show a scaling anomaly, with, for example, the sequences for $\lambda_2^c=0.40$ and $\lambda_2^c=0.78$ converging towards different critical exponents. For $\lambda_2^c\leq 0.30$, a direct study of the minimizing orbits is obstructed, due to their instabilities.

The further extension to scaling along a path with nonzero components in λ_1 *and* λ_2 meets with the same instability problem. Thus some alternative method[6,7] should be tried in order to explore the dependence of the critical exponents on the choice of scaling path.

To conclude, we have found evidence for a scaling anomaly at the critical transition of a simple two-parameter model representing an incommensurate structure. Unless a new kind of critical behavior is involved, our results probably reflect a crossover to a new fixed point under renormalization of the corresponding twist map. However, the exact mechanism which drives the observed scaling behavior remains to be conclusively identified.

We would like to thank F. Axel, R. MacKay, and J. Meiss for valuable comments. This work was supported by Department of Energy Grant No. DE-F-603-85 ER 13402 (J.G.), National Science Foundation Grant No. DMR82-12570 (H.J. and H.S.), and La Jolla Institute Independent Research and Development Funds (B.S.). Funds for use of the San Diege Supercomputer Center were provided by the National Science Foundation. The Center for Studies of Nonlinear Dynamics is affiliated with the University of California, San Diego.

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