Nonanalytic Twist Maps and Frenkel-Kontorova Models

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ABSTRACT

We have studied a class of twist maps and Frenkel-Kontorova (FK) models in which the external potential function is nonanalytic (C^1) and endowed with a variable degree of inflection z . When $z > 3$, recurrence of invariant curves has been observed. An “inverse residue criterion” for the reappearance of an invariant curve — complementary to the “residue criterion” for the disappearance of an invariant curve — is introduced to make a precise determination of the reappearance point. We have also studied the local and global scaling behaviors of these curves. The critical exponents, the singularity spectrum, and the generalized dimensions are found to vary with z when $2 \leq z < 3$, but remain the same for $z \geq 3$. The degree of inflection thus plays a role reminiscent of that of dimensionality in phase transitions with $z = 2$ and 3 corresponding respectively to the lower and upper critical dimensions. When the same nonanalytic function is substituted for the sinusoidal external potential in the standard FK model, the same conclusions are reached: there exists a sequence of pinning-depinning transitions, and the critical exponents of the phonon gap, the coherence length, and the Peierls-Nabarro barrier all show the same dependence on z .

In the summer of 1982 while I (BH) was visiting the Lawrence Berkeley Laboratory, I met Al Lichtenberg and Mike Lieberman. They were then busy preparing the publication of their by-now-famous book Regular and Chaotic Dynamics. They also talked about their work on Arnold diffusion. It was at this point that I became aware of Jeff Tennyson's name. However, I had not had a chance to meet Jeff personally until I returned to Houston from a year's leave at Santa Cruz. I found out that Jeff was at Austin and immediately invited him to come down and give a talk. Jeff gave an excellent talk on his work with John Cary on separatrix crossing. After the talk we went to dinner in a Chinese restaurant. I was impressed both by his work and his amicable personality, so I tried to probe him if he had any interest in seeking a faculty position. Jeff said that he was interested but had already planned to spend one year in Norosibirsk. However, he later returned to Berkeley, and I haven't had a chance to see him since.

Jeff's untimely death has bereft the Hamiltonian community of an original worker. As a token expression of respect, this paper is dedicated to his memory.

1. Introduction

In the context of the standard map the picture of the breakup of an invariant curve is relatively simple. Each rotational curve is characterized by an irrational winding number. These curves serve as barriers to locally stochastic motion. However, as the perturbation strength is increased, more and more of them disappear. At a critical perturbation value, the last invariant curve characterized by the “golden-mean” winding number breaks up and global stochasticity sets in. A “residue criterion” was introduced by Greene¹ to determine the breakup point.

In many respects the breakup of invariant curves is analogous to a phase transition. By utilizing concepts and techniques used in the study of phase transitions, remarkable

progress has been made in the understanding of the breakup of invariant curves.^{2,3}

In phase transitions diverse physical system can be divided into equivalence classes according to certain criteria. These universality criteria are well known in phase transitions. However, much less is known about them in chaotic transitions.⁴

To gain a better understanding of universality in the breakup of invariant curves, we study a class of nonanalytic twist maps:

$$T : \begin{cases} r_{i+1} = r_i - kg(\theta_i), \\ \theta_{i+1} = \theta_i + r_{i+1} \pmod{1}, \end{cases} \quad (1)$$

where $\theta_i \in [-\frac{1}{2}, \frac{1}{2})$ and $r_i \in [0, 1]$. The function $g(\theta) = \theta(1 - |2\theta|^{z-1})$ is nonanalytic (C^1) and is so designed that it has a variable degree of inflection z at the inflection point $\theta = 0$. The motivation for studying such a function is that in the circle map, which can be regarded as the dissipative limit of the standard map, the degree of inflection serves as a universality criterion. The sine function in the circle map possesses a cubic degree of inflection ($z = 3$). To generalize it to an arbitrary degree of inflection, $g(\theta)$ was invented.^{5,6} Although the substitution of this function in the circle map produced no particularly surprising results, many novel features have been discovered in the conservative case.

Many condensed matter systems such as charge density waves, helical magnetic structures in crystals, and monolayers adsorbed on surfaces, exhibit commensurate-incommensurate (CI) phase transitions. A simple theoretical model for studying such transitions is the Frenkel-Kontorova (FK) model⁷ which describes a one-dimensional system of elastically coupled particles subjected to an external periodic potential. By making use of the Kolmogorov-Arnold-Moser theorem, Aubry⁸ pioneered a new and very fruitful approach to this model. The ground states are associated with the orbits of the map. The breakup of an invariant curve represents a phase transition from a sliding phase to

a pinning phase. This pinning transition is similar to a second-order phase transition with well-defined critical exponents^{9,10}. However, when the same nonanalytic function is substituted for the sinusoidal external potential in the standard map, we found that the critical exponents depend on z for $2 \leq z < 3$. For $z > 3$, a sequence of pinning-depinning transitions is observed.

This paper is organized as follows. In Section 2 the recurrence of invariant curves in nonanalytic twist maps and their local as well as global scaling behaviors are studied. The nonanalytic FK model and its critical behavior are studied in Sections 3. In Section 4 some concluding remarks are made.

2. Nonanalytic twist maps^{15,16}

A. Resurrence of invariant curves

For area-preserving twist maps, each orbit is characterized by a winding number ω . ω is rational for a periodic orbit and irrational for an invariant curve. An invariant curve with an irrational winding number ω can be approximated by a sequence of periodic orbits whose winding numbers are the successive convergents of ω . The particular curve we will focus our attention on is the one whose winding number is the inverse of the “golden-mean,” $\omega = (\sqrt{5} - 1)/2$. Its convergents are $\omega_n = F_n/F_{n+1}$, where F_n is a Fibonacci number satisfying $F_{n+1} = F_n + F_{n-1}$ with $F_0 = 0$, $F_1 = 1$. This invariant curve is the most “robust” and is very often the last one to break up. In this paper, we will study the behavior of this critical curve as we vary the degree of inflection.

Since $g(\theta)$ is an odd function, the map (1) is reversible and possesses four symmetry lines:

$$a. \quad \theta = -1/2 \quad (2)$$

$$b. \quad \theta = 0 \quad (3)$$

$$c. \quad \theta = (r - 1)/2 \quad (4)$$

$$d. \quad \theta = r/2. \quad (5)$$

For a rational winding number, each orbit (elliptic or hyperbolic) has two points on two of these four lines. One line will be mapped into another at the half-way point of the orbit. The task of finding a periodic orbit is thus greatly simplified. The following is a summary of our main findings.¹⁵

(1) $k < 0$ or $z \leq 2$

For $k \neq 0$ the residue tends to infinity and the action difference¹¹ tends to a nonzero constant as the period tends to infinity. It suggests that there are no invariant curves when $k \neq 0$. As in the sawtooth map, $k_D = 0$ is the trivial critical point of the breakup of the invariant curve. This is similar to a zero-temperature phase transition.

(2) $2 < z \leq 3$

In this case $k_D \neq 0$; however, no reappearance of invariant curves has been observed. k_D tends to zero monotonically as z decreases from 3 to 2. The phase diagram is shown in Fig. 1. The area below (above) the line indicates the existence (non-existence) of the invariant curve.

(3) $z > 3$

Reappearance of invariant curves¹²⁻¹⁵ has been observed. We found that there is more than one value of k which satisfies Greene's criterion. For example, for $z = 4$, two disappearance points $k_D^{(1)} = 1.4129353$ and $k_D^{(2)} = 1.4261557$ have been found. If an invariant curve disappears at two points, there must be a point k_R , $k_D^{(1)} < k_R < k_D^{(2)}$, at which it reappears. To determine k_R , we introduce an "inverse residue criterion" for the reappearance of an invariant curve:

An invariant curve with a winding number ω that has disappeared at k_D will reappear

at k_R if

$$\lim_{i \rightarrow \infty} R_i^\pm(k) = \begin{cases} \pm\infty, & k < k_R; \\ R^\pm, & k = k_R; \\ 0^\pm, & k > k_R. \end{cases} \quad (6)$$

$R_i^\pm(k)$ are the residues of the minimax (+) and minimizing (−) orbits with winding numbers $\omega_n = P_n/Q_n$ at a given value of k . $|R^\pm| < 1$ are two constants. This “inverse residue criterion” enables us to make a precise determination of the reappearance point. It is complementary to the “residue criterion” for the determination of the disappearance point. For example, for $z = 4$, $k_R^{(1)} = 1.42173415$; and for $z = 6$, $k_R^{(1)} = 1.29946540$, $k_R^{(2)} = 1.45296340$. The superscript “ i ” in $k_{D,R}^{(i)}$ refers to the i th time the invariant curve disappears (D) or reappears (R). We have also computed the action difference and found $\Delta W \rightarrow 0$ if $k < k_D^{(1)}$ or $k_R^{(1)} < k < k_D^{(2)}$; and $\Delta W \rightarrow \text{constant} > 0$ if $k_D^{(1)} < k < k_R^{(1)}$ or $k > k_D^{(2)}$. Fig. 2 shows a typical case. Fig. 3 shows the evolution of the phase portrait from disappearance to reappearance of the invariant curve for the case $z = 6$. In Fig. 3(a), $k < k_D^{(1)}$, the chaotic regions near the period-1 and the period-2 resonances are separated by the invariant curve. In Fig. 3(b), $k_D^{(1)} < k < k_R^{(1)}$, the invariant curve has disappeared and the chaotic regions become connected. In Fig. 3(c), $k_R^{(1)} < k < k_D^{(2)}$, the invariant curve has reappeared and the chaotic regions become separated again. These results together with the critical behavior to be discussed later suggest that $k_R^{(i)}$ are indeed the points at which the invariant curve reappears. Moreover, an invariant curve can recur more than once. For example, for $z = 6$, we have observed that the invariant curve has recurred at least twice. The residues are no longer monotonic functions of k . They tend to infinity right after the invariant curve has disappeared, and become finite again as it reappears. Since we cannot ascertain the existence of a “final” disappearance, the invariant curve can conceivably recur infinitely many times. We have also observed

an exchange of stability before the first breakup of the invariant curve. Fig. 4 shows the variation of the residues with k . It is evident here that stability exchange does not necessarily entail reappearance. When z is a fraction, the dependence of the residues on k is quite complicated. A “bifurcation” of the regions in which the invariant curve exists has also been observed as z varies.

B. Local scaling behavior^{15,16}

The local critical behavior of an invariant curve in the standard map has been well understood by the method of renormalization.^{2,3} One fixed point of the renormalization operator (the simple fixed point), corresponds to the linear map. The other one (the standard fixed point), corresponds to an analytic critical area-preserving twist map. It is known from numerical studies that a broad class of area-preserving twist maps belongs to the same universality class for all quadratic irrationals with the same periodic pattern in the continued fraction expansion. Our results, however, indicate that the critical behavior is much more complicated than expected. We found that the critical exponents of the invariant curve vary with z when $2 \leq z < 3$ but are independent of z when $z \geq 3$. There is a crossover from the simple fixed point to the standard fixed point.

To discuss the critical behavior of the map (1), we first summarize the definitions of various critical exponents. For a pair of minimizing and minimax orbits with a winding number P_n/Q_n , the distance between two neighboring orbit points is $d_n = |\theta_n^{max} - \theta_n^{min}|$, where the superscripts “max” and “min” denote respectively the minimax and minimizing orbits. Period-1 scaling is defined by

$$\begin{aligned} \frac{d_n}{d_{n+1}} &\sim \left(\frac{Q_n}{Q_{n+1}}\right)^{-x^{(1)}}, \\ \frac{r_n - r_{n-1}}{r_{n+1} - r_n} &\sim \left(\frac{Q_n}{Q_{n+1}}\right)^{-y^{(1)}}; \end{aligned} \tag{7}$$

and period-3 scaling

$$\begin{aligned}\frac{d_n}{d_{n+3}} &\sim \left(\frac{Q_n}{Q_{n+3}}\right)^{-x^{(3)}}, \\ \frac{r_n - r_{n-3}}{r_{n+3} - r_n} &\sim \left(\frac{Q_n}{Q_{n+3}}\right)^{-y^{(3)}}.\end{aligned}\tag{8}$$

Due to its better convergence, period-3 scaling is used. For convenience, the exponents on the dominant symmetry line are denoted by $x_s^{(i)}$ and $y_s^{(i)}$, and the exponents on the symmetry line l ($l=a, b, c, d$) are denoted by $x_l^{(i)}$ and $y_l^{(i)}$. In the standard map² it was found that $x_s^{(1)} = 0.721$, $y_s^{(1)} = 2.329$, $x_a^{(3)} = 1.093$, $y_a^{(3)} = 2.329$, and $x_s^{(1)} + y_s^{(1)} = x_a^{(3)} + y_a^{(3)} = 3.05$. The convergence rate of the parameter defines another critical exponent. Again period-3 scaling is used

$$\delta^{(3)} = \frac{k_{n+1} - k_n}{k_{(n+3)+1} - k_{n+3}}.\tag{9}$$

$\delta^{(3)}$ is related to the usual δ by $\delta^{(3)} = \delta^3$. In the standard map $\delta^{(3)} = (1.628)^3$.

For $k < 0$ or $z \leq 2$ the critical point is $k_D = 0$. The system is integrable, and the critical exponents can be calculated analytically: $x = 1$ and $y = 2$. This is just the critical behavior of a linear system. For $2 < z < 3$, we found that the critical exponents at the critical point k_D vary with z (see Table I and Figs. 5-7). For $z = 3$ the critical behavior is the same as that of the standard map. Therefore, the critical behavior changes from that of the linear map to that of the standard map as z varies from 2 to 3. The sum of the exponents, $x + y$, which is a more useful quantity in the study of transport, shows a slightly increasing trend. However, the increase is too small to exclude the possibility that it is in fact a constant. Since δ decreases with z , higher-period orbits are needed to compute the exponents. As z is close to 2, the convergence of δ_n towards δ is slowed down, and the exponents are very hard to compute. When $z \geq 3$, the exponents at the disappearance and reappearance points are equal and the same as those of the standard map. They are independent of z (see Table II). In this sense the degree of inflection z

plays a role quite similar to that of dimensionality in phase transitions with $z = 2$ and 3 corresponding respectively to the lower and upper critical dimensions.

C. Global scaling behavior^{16,17}

At the critical point, the invariant curve loses its analyticity and breaks up into a Cantor set called a “cantorus”. The full complexity of its scaling structure can be described only by a spectrum of critical exponents α and their densities $f(\alpha)$, of which the exponents x and y comprise only a part.¹⁹ To compute $f(\alpha)$ we divide the curve into pieces labeled by an index i which runs from 1 to N . The size of the i th piece is l_i and the density of points in l_i is p_i . α is defined by $p_i = l_i^\alpha$. It lies in an interval $[\alpha_{min}, \alpha_{max}]$, the endpoints of which are determined by the local scaling behavior. $f(\alpha)$ is the Hausdorff dimension of the set of points having exponent α .

To calculate $f(\alpha)$ of the cantorus, we follow the formalism described in Ref. 19. A periodic orbit with a winding number $\omega_n = F_{n-1}/F_n$, is divided into $N = F_n$ pieces consisting of two nearby orbit points. The Euclidean distance between these two points $l_i(n) = \sqrt{(\tau_i - \tau_{i+F_{n-1}})^2 + (\theta_i - \theta_{i+F_{n-1}})^2}$ defines a natural scale for the partition with a measure $p_i = 1/F_n$. Then a partition function can be defined

$$\Gamma_n(q, \tau) = \sum_{i=1}^{F_n} \frac{p_i^q}{l_i^\tau} = F_n^{-q} \sum_{i=1}^{F_n} l_i^{-\tau}. \quad (10)$$

For an asymptotically recursive structure, the partition function is of order unity when

$$\tau = (q - 1)D_q. \quad (11)$$

D_q is a set of generalized dimensions, of which D_0 is the Hausdorff dimension, D_1 the information dimension, and D_2 the correlation dimension. The spectrum $f(\alpha)$ is defined by the Legendre transformation of $\tau(q)$,

$$\alpha(q) = \frac{d\tau}{dq}, \quad (12)$$

$$f(q) = q\alpha(q) - \tau. \quad (13)$$

Eliminating q gives the function $f(\alpha)$. To improve the convergence of $f(\alpha)$ as $\omega_n \rightarrow \omega$, one can employ the usual ratio trick

$$\frac{\Gamma_n(q, \tau)}{\Gamma_{n-1}(q, \tau)} = 1 \quad (14)$$

For the map (1), we will use period-3 ratio due to its better convergence

$$\frac{\Gamma_n(q, \tau)}{\Gamma_{n-3}(q, \tau)} = 1. \quad (15)$$

From Eq. (12), q and α can be calculated as functions of τ

$$q = \frac{1}{\ln\left(\frac{F_{n-1}}{F_n}\right)} \left[\ln\left(\sum_{i=1}^{F_{n-1}} l_i^{-\tau}(n-1)\right) - \ln\left(\sum_{i=1}^{F_n} l_i^{-\tau}(n)\right) \right] \quad (16)$$

$$\alpha = \ln\left(\frac{F_{n-1}}{F_n}\right) \left[\frac{\sum_{i=1}^{F_n} l_i^{-\tau}(n) \ln(l_i(n))}{\sum_{i=1}^{F_n} l_i^{-\tau}(n)} - \frac{\sum_{i=1}^{F_{n-1}} l_i^{-\tau}(n-1) \ln(l_i(n-1))}{\sum_{i=1}^{F_{n-1}} l_i^{-\tau}(n-1)} \right]^{-1} \quad (17)$$

We have calculated $f(\alpha)$ at the disappearance and reappearance points for a variety of values of z . The $f(\alpha)$ curves are the same as that of the standard map²⁰ and are independent of z for $z \geq 3$, but they vary with z for $2 \leq z < 3$. Fig. 8 plots the $f(\alpha)$ curves for $2 \leq z \leq 3$. It shows that as z varies from 3 to 2, the $f(\alpha)$ curves shrink from that of the standard map to that of the linear case. Fig. 9 plots D_q versus q for $2 \leq z \leq 3$. For $z = 2$, the critical case has a trivial scaling with a single dimension $D = 1$. For $z = 3$, the critical case is the same as that of the standard map which has a set of fractal dimensions lying in the interval $[D_{-\infty}, D_{\infty}]$. As z varies from 3 to 2, the critical invariant curve changes smoothly from a cantor set characterized by the standard fixed point to a smooth curve characterized by the simple fixed point.

The endpoints of the $f(\alpha)$ curves can be determined exactly in terms of the local critical exponents. In the partition function (10), as $q \rightarrow -\infty$, the dominant contribution comes from the largest l_{max} , corresponding to the most rarefied region of the cantor set;

as $q \rightarrow \infty$, the dominant contribution comes from the smallest $l_{\min}$, corresponding to the most concentrated region of the cantorus. The most rarefied region is on the dominant symmetry line, and the most concentrated region is on one of the nondominant symmetry lines. For $2 < z < 3$, they are $\theta = 0$ and $\theta = -1/2$. Therefore, from Eq. (15),

$$\lim_{q \rightarrow -\infty} \frac{\Gamma_n}{\Gamma_{n-3}} = \lim_{q \rightarrow -\infty} \left(\frac{F_n}{F_{n-3}} \right)^{-q} \left(\frac{d_n(0)}{d_{n-3}(0)} \right)^{-\tau}, \quad (18)$$

$$\lim_{q \rightarrow \infty} \frac{\Gamma_n}{\Gamma_{n-3}} = \lim_{q \rightarrow \infty} \left(\frac{F_n}{F_{n-3}} \right)^{-q} \left(\frac{d_n(-\frac{1}{2})}{d_{n-3}(-\frac{1}{2})} \right)^{-\tau}. \quad (19)$$

Together with Eq. (8), we obtain,

$$\alpha_{\max} = D_{-\infty} = \frac{1}{x_b^{(3)}}, \quad (20)$$

$$\alpha_{\min} = D_{\infty} = \frac{1}{x_a^{(3)}}. \quad (21)$$

In Table I, the variation of $\alpha_{\max}$ and $\alpha_{\min}$ with z is listed for $2 \leq z \leq 3$. Excellent agreement with those obtained from the $f(\alpha)$ curves can be seen.

3. Nonanalytic Frenkel-Kontorova model¹⁸

The Hamiltonian of the FK model can be written as

$$\phi(\{u_i\}) = \sum_i \left[\frac{1}{2}(u_{i+1} - u_i)^2 + kV(u_i) - \mu(u_{i+1} - u_i) \right], \quad (22)$$

where u_i denotes the position of the i th particle, μ the tensile strength and k the amplitude of the external periodic potential V . In the standard FK model $V(u_i)$ is a sinusoidal function. Physically the most interesting configuration $\{u_i\}$ is the ground state which has the minimum energy for a given boundary condition and satisfies the equilibrium condition

$$\frac{\partial \phi}{\partial u_i} = -u_{i+1} + 2u_i - u_{i-1} + k \frac{\partial V}{\partial u_i} = 0. \quad (23)$$

By setting $r_i = u_i - u_{i-1}$ as the conjugate variable of u_i , Eq. (23) generates an area-preserving twist map. The ground states of the FK model are related therefore to orbits

of its associated map. For the standard FK model, this associated map is just the standard map. It was shown that the ground state is either periodic or quasiperiodic.²¹ The winding number ω of these orbits corresponds to the mean particle distance of ground states. When ω is a rational number, the ground state is commensurate and corresponds to a minimizing periodic orbit; when ω is an irrational number, the ground state is incommensurate and corresponds to a quasiperiodic orbit. Here we are interested in the incommensurate states. In the standard FK model, as the parameter k varies, an incommensurate state undergoes a structural phase transition at a well-defined critical value k_c . For $k < k_c$, the chain of particles responds smoothly to an infinitesimal displacing force: it is called a sliding phase; for $k > k_c$ the particles become locked to their positions: it is called a pinned phase. This transition is connected to the breakup of an invariant curve with the sliding phase represented by an invariant curve and the pinned phase by a cantor. This pinning transition is similar to a second-order phase transition with well-defined critical exponents.^{9,10}

To study the problem of universality in FK models, we substitute the sinusoidal external potential with the following potential

$$V(u_i) = \frac{1}{2}\theta_i^2 \left(1 - \frac{2}{z+1}|2\theta_i|^{z-1}\right) \quad , \quad \theta_i = u_i \pmod{1} \quad (24)$$

where $\theta_i \in [-\frac{1}{2}, \frac{1}{2})$. $V(u_i)$ is periodically extended

$$V(\theta_i) = V(\theta_i + 1) \quad . \quad (25)$$

Fig. 10 shows $V(u_i)$ given in Eq. (24) for some values of z as well as the sinusoidal potential of the standard FK model. For this class of nonanalytic FK models

$$\left. \frac{\partial^3 V}{\partial \theta_i^3} \right|_{\theta_i=\frac{1}{2}} \neq \left. \frac{\partial^3 V}{\partial \theta_i^3} \right|_{\theta_i=-\frac{1}{2}} \quad . \quad (26)$$

The associated maps of these nonanalytic FK models are the nonanalytic twist maps of

Eq. (1). The reappearance of an invariance curve in map (1) results in a transition from a pinned phase to a sliding phase, called a depinning transition. For $z > 3$, the recurrence of invariant curves thus represents a sequence of pinning-depinning transitions. They may be relevant to physical systems exhibiting a sequence of metal-insulator transitions¹². To investigate the critical behavior of the pinning and depinning transitions, we will study the gap in the phonon spectrum, the coherence length, and the Peierls-Nabarro barrier of the ground state.

A. The Gap in the Phonon Spectrum

Consider an infinitesimal particle displacement $\{\epsilon_i\}$ around an equilibrium configuration $\{u_i\}$. The Hamiltonian (22) can be expanded to second order in ϵ_i , [the first order term vanishes due to Eq. (23)].

$$\phi(\{u_i + \epsilon_i\}) = \phi(\{u_i\}) + \delta^2\phi , \quad (27)$$

where

$$\delta^2\phi = \frac{1}{2} \sum_i \left[\left(2 + k \frac{\partial^2 V}{\partial u_i^2} \right) \epsilon_i^2 - 2\epsilon_{i+1}\epsilon_i \right] . \quad (28)$$

The physical stability (metastability) of an equilibrium configuration of Eq. (23) requires that $\delta^2\phi$ be a positive quadratic form in $\{\epsilon_i\}$. The equation of small-amplitude vibrations of the particles around their equilibrium positions can be derived from Eq. (28)

$$\ddot{\epsilon}_i(t) = -\epsilon_{i+1}(t) - \epsilon_{i-1}(t) + \left(2 + \frac{\partial^2 V}{\partial u_i^2} \right) \epsilon_i(t) , \quad (29)$$

where the mass of the particles is taken to be unity. The time Fourier transform of Eq. (29) is

$$\Omega^2 \epsilon_i(\Omega) = -\epsilon_{i+1}(\Omega) - \epsilon_{i-1}(\Omega) + \left(2 + \frac{\partial^2 V}{\partial u_i^2} \right) \epsilon_i(\Omega) . \quad (30)$$

This equation determines the phonon eigenfrequencies Ω_e and the corresponding eigenmodes $\{\epsilon_i^e\}$. For the ground state, all the eigenvalues Ω_e^2 are positive or zero because of

the positive-definiteness of Eq. (28). The gap in the phonon spectrum Ω_G is defined as the positive square root of the smallest eigenvalue, i.e. the lowest phonon frequency.

In the sliding phase with mean particle distance ω the position of the i th particle can be parametrized as $u_i = u(i\omega + \alpha)$ where u is the so-called hull function. u is differentiable and α is an arbitrary phase.²¹ Inserting this function into Eq. (23) and differentiating it with respect to α shows that

$$\epsilon_i = u'(i\omega + \alpha) \quad (31)$$

is a solution of Eq. (30) with $\Omega^2 = 0$. Consequently in the sliding phase the gap in the phonon spectrum vanishes.

In contrast, in the pinned incommensurate phase the hull function becomes discontinuous with a derivative which is zero almost everywhere. Thus Eq. (31) no longer defines an eigenmode for Eq. (30) and Ω_G does not necessarily vanish. Numerical results on the standard FK model^{9,10} indicate that Ω_G behaves as

$$\Omega_G(k) \sim (k - k_c)^\chi . \quad (32)$$

Numerically, $\chi \approx 1.02$.

We have studied the phonon spectrum in the nonanalytic FK model. The mean particle distance is still chosen to be the “golden-mean.” The pinned “golden-mean” incommensurate phase can be approximated by a sequence of minimizing orbits with winding numbers $\omega_n = F_{n-1}/F_n$. For each ω_n , Eq. (30) is a system of F_n linear equations,

which can be written in the matrix form

$$\Omega^2 \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \vdots \\ \vdots \\ \epsilon_{F_n} \end{pmatrix} = \begin{pmatrix} b_1 & -1 & 0 & 0 & \dots & \cdot & 0 \\ -1 & b_2 & -1 & 0 & \dots & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -1 \\ 0 & \dots & 0 & -1 & b_{F_n} \end{pmatrix} \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \vdots \\ \vdots \\ \epsilon_{F_n} \end{pmatrix}, \quad (33)$$

where

$$b_i = 2 - k[1 - (z + 1)|2\theta_i|^z], \quad \theta_i = u_i \pmod{1}. \quad (34)$$

The phonon spectrum can be computed by diagonalising this matrix. However, the computation is complicated by the instability of minimizing orbits and the proliferation of nearby nonminimizing orbits with the same winding numbers as a result of bifurcation. To identify a minimizing orbit we start in the subcritical (supercritical) region of the pinning (depinning) transition where the orbits are dispersed and easy to locate. We then extrapolate to obtain an estimate for a larger (smaller) value of k . Sufficiently close to the transition this method is very effective. Fitting the data of Ω_G versus $|k - k_c|$ in a log-log plot, we found that the power law Eq. (32) is valid provided that k is not too close to k_c . For $z \geq 3$ the critical exponent χ in the pinning and depinning transitions is the same as that in the pinning transition in the standard FK model. For $2 \leq z < 3$, there is only a pinning transition and χ is found to depend on z . Fig. 11 shows Ω_G as a function of k for different values of $2 < z \leq 3$. To plot all these curves with different z in one figure, the abscissa is chosen to be $(k - k_c)/(k_1 - k_c)$ where k_1 is the value of k at which $\Omega_G = 0.01$. For $k > k_c$, the increase of Ω_G with k indicates the appearance of a pinned phase. Due to the finite size of the system ($l = 987/1597$ in the figures), Ω_G cannot exactly go to zero as $k \rightarrow k_c$. In the next section we will discuss why in the

close vicinity of the critical point larger systems are needed for better results. Fig. 12 shows the variation of χ with z for $2 \leq z \leq 3$. As z decreases from 3 to 2, χ increases monotonically from the lower bound of $\chi = 1.02$, which is that of the standard FK model, to the upper bound of $\chi \approx 5$ at $z = 2$. Since as z gets close to 2 the computation becomes quite delicate, the value of χ at $z = 2$ was obtained by extrapolation.

B. The Coherence Length

The coherence length of the ground state measures the range of the perturbation along the chain when one of particles (assumed at site 0) is perturbed from its equilibrium position u_0 to a new position $u_0 + \delta u_0$. As this perturbation propagates along the lattice, the position of a particle originally at u_n becomes $u_n + \delta u_n$ in the new metastable configuration. Generally the deviation δu_n decreases exponentially

$$\delta u_n \sim \delta u_0 \exp(-|n|/\xi) , \quad (35)$$

which defines the coherence length ξ of the ground state. Since the perturbed configuration $\{u_n + \delta u_n\}$ also satisfies the equilibrium equation, expanding Eq. (23) to first order in δu_n gives

$$-\delta u_{n+1} - \delta u_{n-1} + \left(2 + \frac{\partial^2 V}{\partial u_n^2}\right) \delta u_n = 0. \quad (36)$$

This equation is identical to Eq. (30) with $\Omega = 0$ and thus for a sliding phase we have a solution of Eq. (36)

$$\delta u_n = \frac{\delta u_0}{u'(\alpha)} u'(nl + \alpha) . \quad (37)$$

In the sliding phase the hull function $u(x)$ is differentiable and strictly increasing;²¹ therefore, $u'(x)$ is a positive continuous function and δu_n does not go to zero as $n \rightarrow \infty$. Thus in this case $\xi = \infty$ and the sliding phase is a phason mode in which the perturbation propagates to infinity without any restoring force.

By setting $\delta\theta_n = \delta u_n$ and $\delta r_n = \delta\theta_n - \delta\theta_{n-1}$, Eq. (36) yields the linearized map of map (1)

$$(\delta r_n, \delta\theta_n) = LT^n(\delta r_0, \delta\theta_0) \quad (38)$$

where LT is the Jacobian matrix of T . A minimizing periodic orbit representing a minimum energy configuration is dynamically unstable and has a pair of reciprocal eigenvalues λ and λ^{-1} . As these minimizing convergents approach a cantorus (pinned incommensurate phase), λ goes to infinity. Thus in the limit $|n| \rightarrow \infty$, $LT^n(\delta r_0, \delta\theta_0)$ diverges as $\exp(\gamma|n|)$ in the expansion direction and converges as $\exp(-\gamma|n|)$ in the contraction direction, where γ is the Lyapunov exponent of the orbit

$$\gamma = \lim_{n \rightarrow \infty} \frac{\ln \lambda}{n} \quad (39)$$

The contraction direction corresponds to the physical solution. A comparison with Eq. (35) shows that the coherence length of the ground state is the inverse of the Lyapunov exponent of the corresponding orbit of the map (1)

$$\xi = \frac{1}{\gamma} \quad (40)$$

In a pinned incommensurate phase, the particles are locked to their positions and thus the coherence length is finite. In the sliding phase, in contrast, the chain of particles slides freely under an infinitesimal displacing force and therefore ξ is infinite. As $k \rightarrow k_c$ in a pinned incommensurate phase

$$\xi \sim |k - k_c|^{-\nu} \quad (41)$$

In the standard FK model, $\nu \approx 1.0$.

We have studied the coherence length of the pinned phase both in the pinning and depinning transitions. The same method discussed above was used to track the minimizing orbits which form the convergents of the “golden-mean” curve. In Fig. 13 we plot

the variation of γ versus $(k - k_c)/(k_1 - k_c)$ for $2 < z \leq 3$, where k_1 is the value of k at which $\gamma = 0.01$. It is seen that γ is different from zero in the pinned phase due to the finite size of the system ($\omega = 987/1597$). In the vicinity of the transition point, γ is small and ξ is thus significant. As a consequence, finite size effects are perceptible close to the transition point in the numerical computation. To lessen finite size effects the size of the system (i.e. period of the orbit) should be much larger than the coherence length. From Fig. 13 it can also be seen that, in the vicinity of k_c , the smaller z , the smaller γ . For instance, at $(k - k_c)/(k_1 - k_c) = 0.1$, the coherence length $\xi \approx 1000$ for $z = 3$ and $\xi \approx 4000$ for $z = 2.1$. Therefore, as z approaches 2, much larger sizes are needed, which render the computation harder to perform. The results, however, can be judged by studying the convergence of the successive commensurate configurations which form the convergents of the incommensurate configuration. Fig. 14 is an example in which we plot γ as a function of $k - k_c$ for $\omega = 610/987$ and $987/1597$ with $z = 1.8$. It is shown that when $k - k_c > 0.01$ the data computed from the orbit of $\omega = 987/1597$ are quite reliable.

A fit of the obtained data of γ to a log-log plot again yields a power-law behavior

$$\gamma(k) \sim |k - k_c|^\nu . \quad (42)$$

For $z \geq 3$ the exponent ν is the same as that of the standard FK model. For $2 \leq z < 3$ ν varies with z (see Fig. 15). As z decreases from 3 to 2, ν increases monotonically from the lower bound of $\nu = 1.0$, the value of the standard FK model, to the upper bound of $\nu \approx 6$ at $z = 2$. As before, the value of χ at $z = 2$ was obtained by extrapolation.

C. Peierls-Nabarro Barrier

The Peierls-Nabarro (PN) barrier of the ground state is defined as the smallest energy barrier that must be overcome to translate continuously the chain of particles over the

external potential⁸. In the sliding phase the chain can slide without any extra energy. In this case the translation of the incommensurate structure can be obtained by shifting continuously the phase α in the hull function. Due to the continuity of the hull function the motion of each particle is continuous. Since the energy of the system is independent of α , the PN barrier vanishes in the sliding phase. This is no longer the case in the pinned phase where the ground state is represented by a cantor set which is a Cantor set with a dense set of gaps. Given a minimizing periodic orbit $\{\theta_i|i = 1, \dots, Q_n\}$ which approximates a cantor set, we define $\{\theta'_i|i = 1, \dots, Q_n\}$ to be the same orbit but with the points relabeled so that θ'_i is the closest point to the right of θ_i . In the limit $Q_n \rightarrow \infty$, a shift of $\{\theta_i|i = 1, \dots, Q_n\}$ to $\{\theta'_i|i = 1, \dots, Q_n\}$ thus represents a continuous translation of the chain. However, as we know, between two nearby minimizing orbits there is a minimax orbit which has the same winding number but a maximum energy. Thus in the shift of $\{\theta_i|i = 1, \dots, Q_n\}$ to $\{\theta'_i|i = 1, \dots, Q_n\}$ one must pass through this minimax orbit. It follows that the PN barrier ϕ_{PN} is the difference in energies between the minimax and minimizing orbits, i.e.

$$\phi_{PN} = \lim_{n \rightarrow \infty} [\phi_{max}(\omega_n) - \phi_{min}(\omega_n)] , \quad (43)$$

where $\phi_{max}(\omega_n)$ [$\phi_{min}(\omega_n)$] is respectively the energy of the minimax (minimizing) orbit with winding number ω_n . Eq. (43) gives an effective tool for studying the PN barrier of the pinned incommensurate phase in both the pinning and depinning transitions. In Fig. 16 the variation of ϕ_{PN} versus $(k - k_c)/(k_1 - k_c)$ for $2 < z \leq 3$ is plotted, where k_1 is the value of k at which $\phi_{NP} = 1.6 \times 10^{-8}$. Here the winding number of the orbits is 987/1597. Fitting the data to a log-log plot shows that the PN barrier behaves as

$$\phi_{PN} \sim |k - k_c|^\psi . \quad (44)$$

For $z \geq 3$, $\psi = 3.01$, in agreement with that of the standard FK model. However, as z

varies from 3 to 2, ψ increases monotonically from the lower bound of $\psi = 3.01$ at $z = 3$ to the upper bound of $\psi \approx 16$ at $z = 2$, which was again estimated by extrapolation (see Fig. 17).

D. Scaling Relations

A comparison of Figs. 12, 15, and 17 shows that all three exponents χ , ν , and ψ have the same general behavior along the critical line. If we make a scale change in the vertical axis, the three curves almost coincide. This indicates that there may exist a scaling relation among them. For the standard FK model Peyard and Aubry conjectured that⁹

$$2\chi + \nu = \psi \quad . \quad (45)$$

To check this conjecture we have listed the values of ψ , χ and ν and calculated the deviation $D = |\psi - (2\chi + \nu)|$ and relative deviation $RD = |\psi - (2\chi + \nu)|/[0.5(\psi + 2\chi + \nu)]$ (see Table III). For $z = 3$ the deviation and relative deviation are only 0.02 and 0.65%, but it is weakly violated for $2 < z < 3$. However, as z decreases from 3 to 2, the deviation gets larger. The worst case is $z = 2.1$, where the deviation and relative deviation are 0.7 and 5.4% respectively. Recently, Mackacy³ claimed that the correct scaling relation should be

$$2\chi + \nu = \psi + \eta' \quad , \quad (46)$$

where $\eta' \simeq 0.029$ is a subcritical scaling exponent.

4. Concluding remarks

The study undertaken here has revealed surprisingly rich and novel critical behaviors of invariant curves. Their life story is by far more complicated than hitherto thought of. They can reappear after have disappeared. The degree of inflection plays a role very similar to that of dimensionality in phase transitions. The critical exponents depend on

the degree of inflection between a lower and upper critical values. As a result of the recurrence of invariant curves, the nonanalytic FK model exhibits a sequence of pinning and depinning transitions when $z > 3$. This phenomenon may be relevant to physical systems exhibiting a sequence of metal-insulator transitions. All these unexpected new features suggest that one should undertake a more detailed study of the behavior of invariant curves.^{22,23} Such a study will lead to not only a more complete understanding of invariant curves but also their application to real physical systems.

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Table I. The critical points k_D , the critical exponents and the endpoints of the $f(\alpha)$ curves for $2 \leq z \leq 3$. $x_i^{(3)}$ and $y_i^{(3)}$ are the exponents on the dominant symmetry line for $i = b$ and the nondominant symmetry line for $i = a$ respectively.

z	k_D	$\delta^{(3)}$	$x_a^{(3)}$	$y_a^{(3)}$	$x_a^{(3)} + y_a^{(3)}$	$x_b^{(3)}$	$y_b^{(3)}$	$x_b^{(3)} + y_b^{(3)}$	α_{min}	α_{max}
2.0	0	—	1	2	3	1	2	3	1	1
2.1	0.219	1.27	1.021	1.978	2.999	0.965	2.036	3.001	0.979	1.036
2.2	0.391	1.42	1.032	1.969	3.001	0.935	2.067	3.002	0.969	1.070
2.3	0.5375	1.55	1.040	1.963	3.003	0.907	2.098	3.005	0.962	1.103
2.4	0.6617	1.75	1.047	1.958	3.005	0.881	2.127	3.008	0.955	1.135
2.5	0.76828	1.97	1.053	1.956	3.009	0.858	2.155	3.013	0.950	1.166
2.6	0.86037	2.23	1.060	1.954	3.014	0.835	2.181	3.016	0.943	1.198
2.7	0.94034	2.53	1.068	1.952	3.020	0.810	2.211	3.021	0.936	1.235
2.8	1.010114	2.88	1.075	1.950	3.025	0.788	2.239	3.027	0.930	1.269
2.9	1.071375	3.36	1.084	1.950	3.034	0.763	2.271	3.034	0.923	1.311
3.0	1.125454	4.25	1.100	1.947	3.047	0.721	2.330	3.051	0.909	1.387

Table II. The disappearance (k_D) and reappearance (k_R) points and the critical exponents for $z > 3$.

z	k	$x_s^{(3)}$	$y_s^{(3)}$	$x_s^{(3)} + y_s^{(3)}$	$x_n^{(3)}$	$y_n^{(3)}$	$x_n^{(3)} + y_n^{(3)}$
3.8	$k_D^{(1)} = 1.38253450$	0.7284	2.3261	3.0545	1.0990	1.9448	3.0438
	$k_R^{(1)} = 1.38760367$	0.7226	2.3295	3.0521	1.1018	1.9512	3.0530
4	$k_D^{(1)} = 1.41293530$	0.7219	2.3287	3.0506	1.1045	1.9419	3.0464
	$k_R^{(1)} = 1.42173415$	0.7223	2.3281	3.0504	1.1015	1.9466	3.0481
	$k_D^{(2)} = 1.42615570$	0.7203	2.3329	3.0533	1.0986	1.9425	3.0412
5	$k_D^{(1)} = 0.80993000$	0.7234	2.3281	3.0515	1.1030	1.9432	3.0462
	$k_R^{(1)} = 1.05287350$	0.7216	2.3288	3.0504	1.1040	1.9432	3.0472
	$k_D^{(2)} = 1.39647420$	0.7221	2.3285	3.0505	1.1044	1.9422	3.0466
	$k_D^{(1)} = 0.70400046$	0.7218	2.3289	3.0507	1.1046	1.9421	3.0467
6	$k_R^{(1)} = 1.29946540$	0.7227	2.3284	3.0511	1.1037	1.9432	3.0470
	$k_D^{(2)} = 1.43731867$	0.7228	2.3304	3.0532	1.1121	1.9327	3.0448
	$k_R^{(2)} = 1.45296340$	0.7229	2.3303	3.0533	1.1121	1.9326	3.0447
	$k_D^{(3)} = 1.51257548$	0.7221	2.3293	3.0513	1.1024	1.9454	3.0478
11	$k_D^{(1)} = 0.27830553$	0.7211	2.3303	3.0515	1.1021	1.9462	3.0483

Table III. Variation of the phonon gap exponent χ , the coherence length exponent ν and the Peierls-Nabarro barrier exponent ψ with z for $2 < z \leq 3$. The deviation and relative deviation of Eq. (45) are, respectively, $D = |\psi - (2\chi + \nu)|$ and $RD = |\psi - (2\chi + \nu)|/[0.5(\psi + 2\chi + \nu)]$.

z	χ	ν	ψ	$2\chi + \nu$	D	RD (%)
3.0	1.02	1.0	3.06	3.04	0.02	0.65
2.9	1.17	1.15	3.54	3.48	0.06	1.7
2.8	1.31	1.32	4.04	3.94	0.1	2.5
2.7	1.45	1.51	4.57	4.42	0.15	3.3
2.6	1.68	1.73	5.20	5.09	0.11	2.1
2.5	1.93	2.02	6.09	5.88	0.21	3.2
2.4	2.25	2.39	7.10	6.89	0.21	2.8
2.3	2.67	2.88	8.53	8.22	0.31	3.7
2.2	3.24	3.7	10.5	10.2	0.3	2.9
2.1	4.0	4.7	13.4	12.7	0.7	5.4

Figure captions:

Fig. 1. The critical value k_D as a function of z for $2 \leq z \leq 3$. The area below (above) the critical line indicates the existence (non-existence) of the “golden-mean” invariant curve.

Fig. 2. The action difference ΔW as a function of k for $z = 4$ and $(Q_i, P_i) = (1597, 987)$.

Fig. 3. The phase portraits of the invariant curve from disappearance to reappearance for the case $z = 6$. 1, 2 and G indicate respectively the period-1 resonance, period-2 resonance and the “golden-mean” invariant curve. (a) $k = 0.704 < k_D^{(1)}$; (b) $k_D^{(1)} < k = 0.9 < k_R^{(1)}$; (c) $k_R^{(1)} < k = 1.35 < k_D^{(2)}$.

Fig. 4. The residues R_i of the initially elliptic orbits for $z = 5$. (a) $(Q_i, P_i) = (233, 144)$; (b) $(377, 233)$; (c) $(610, 377)$. The residues of the initially hyperbolic orbits are symmetrically located and are not shown. Stability exchange occurs before the first breakup of the invariant curve for (a), but not for (b) and (c).

Fig. 5. The parameter scaling exponent $\delta^{(3)}$ as a function of z for $2 \leq z \leq 3$.

Fig. 6. The critical exponents on the dominant symmetry line $x_s^{(3)}$ and the nondominant symmetry line $x_c^{(3)}$ as a function of z for $2 \leq z \leq 3$.

Fig. 7. The critical exponents on the dominant symmetry line $y_s^{(3)}$ and the nondominant symmetry line $y_c^{(3)}$ as a function of z for $2 \leq z \leq 3$.

Fig. 8. The singularity spectrum $f(\alpha)$ of the critical invariant curve for $2 \leq z \leq 3$. The number on the curve indicates the value of z .

Fig. 9. The generalized dimensions D_q of the critical invariant curve for $2 \leq z \leq 3$. The number on the curve indicates the value of z .

Fig. 10. External periodic potentials of the standard and nonanalytic FK models. (a)

$z = 2$; (b) the sinusoidal potential; (c) $z = 2.5$; (d) $z = 3$; (e) $z = 4$.

Fig. 11. The gap in the phonon spectrum Ω_G as a function of k for different values of $z \in (2, 3]$. k_c is the pinning transition point and k_1 the value of k at which $\Omega_G = 0.01$. The number on the curve indicates the value of z .

Fig. 12. The critical exponent χ of the gap in the phonon spectrum as a function of z for $z \in [2, 3]$.

Fig. 13. The Lyapunov exponent γ of the pinned state as a function of k for different values of $z \in (2, 3]$. k_c is the pinning transition point and k_1 the value of k at which $\gamma = 0.01$. The number on the curve indicates the value of z .

Fig. 14. γ as the function of $k - k_c$ calculated from two systems with different sizes. The upper one has $\omega = 610/987$ and the lower one $\omega = 987/1597$.

Fig. 15. The critical exponent ν of the coherence length as a function of z for $z \in [2, 3]$.

Fig. 16. The PN barrier ϕ_{PN} as a function of k for different values of $z \in (2, 3]$. k_c is the pinning transition point and k_1 the value of k at which $\phi_{PN} = 1.6^{-8}$. The number on the curve indicates the value of z .

Fig. 17. The critical exponent ψ of the PN barrier as a function of z for $z \in [2, 3]$.

Fig. 1

Fig 1

Fig. 2

Fig. 3(a)

Fig 3(b)

Fig 3(c)

Fig. 4

Fig. 5

FIG. 6

FIG. 7

Fig. 8

Fig. 9

Fig. 1

Fig. 10

Fig. 11

Fig. 12

Fig. 13

Fig. 15

Fig. 17