Pinning transition of the discrete sine-Gordon equation

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The ground state of the discrete sine-Gordon equation, used to model a one-dimensional solid in a periodic potential, is examined in the incommensurate region. The behavior of the system near the transition from an unpinned to a pinned phase (first discussed by Aubry) is investigated. A disorder parameter and a correlation length are defined and shown numerically to obey scaling relations on both sides of the transition. The system studied is equivalent to the "standard map" of dynamical systems theory, and this relationship is discussed. In particular, our results extend the scaling behavior found by Shenker and Kadanoff into the "chaotic" regime.

I. INTRODUCTION

Many solid-state systems, among them charge-density waves, adsorbed monolayers, and incommensurate alloy structures, exhibit competing periodicities.[1] Quasiperiodic states also arise in many dynamical systems and have been extensively studied recently, both experimentally and theoretically.[2]

In this paper we examine a model system which displays a transition between two types of incommensurate ground states. This simple, classical one-dimensional model is a collection of balls connected by Hooke's-law springs between nearest neighbors all sitting in a sinusoidal substrate potential at zero temperature. This model (the discrete sine-Gordon equation) was introduced nearly 50 years ago by Frenkel and Kontorova.[3] The potential energy of the system is

$$U=\tfrac{1}{2}K\sum_j (Z_{j+1}-Z_j-a)^2-\bar{V}\sum_j \cos\left[\frac{2\pi}{b}Z_j\right] . \tag{1.1}$$

Here Z_j is the position in space of the jth ball, a the equilibrium length of each spring, b the period of the substrate potential, K the spring constant, and $\bar{V}$ the depth of the substrate wells.

The force on the jth ball is

$$f_j=K(Z_{j+1}-2Z_j+Z_{j-1})-\frac{2\pi}{b}\bar{V}\sin\left[\frac{2\pi}{b}Z_j\right] . \tag{1.2a}$$

We look for equilibrium positions of the balls, which involves solving the set of equations

$$f_j=0 \tag{1.2b}$$

for all j. We will particularly be concerned with the ground states of the system, rather than general extrema of the energy.

This system has been studied in some detail.[4] Frank and van der Merwe[5] solved the continuum approximation to (1.2) and found solutions that correspond to solitons. More recently, Aubry[6] has studied the discrete model; we will describe and interpret some of his results.

We note that Eqs. (1.2) may be rewritten in a simpler form (which we will use henceforth) by rescaling the variables

$$X_j=\frac{2\pi}{b}Z_j ,$$

$$V=\left[\frac{2\pi}{b}\right]^2\frac{\bar{V}}{K} ,$$

to yield

$$X_{j+1}-2X_j+X_{j-1}-V\sin X_j=0 . \tag{1.3}$$

We wish to investigate properties of the ground state of the balls and, in addition, the effects of a uniform applied force (caused by, for example, tipping the corrugated table on which the balls rest, if the potential is gravitational). In particular, for an infinitesimally small force, under some conditions the balls roll down the incline, while in other situations they remain stuck in the wells. The first case we call "unpinned" and the second "pinned." We will show in the next section that whether or not the balls are pinned depends on the phonon spectrum of the system with no applied force. As we shall see, if a zero-frequency phonon exists, the balls roll; otherwise they are pinned.

A set of equations equivalent to Eqs. (1.2) and (1.3) also have been studied from a dynamical systems point of view where the spatial index j is thought of as time. By defining

$$\theta_j=X_j ,$$

$$r_j=X_j-X_{j-1} ,$$

Eq. (1.3) can be written as discrete time (j) evolution equations

$$r_{j+1}=r_j+V\sin\theta_j \ , \quad (1.4a)$$

$$\theta_{j+1}=\theta_j+r_{j+1} \ , \quad (1.4b)$$

which are the defining equations for the so-called standard map.

This map is a model for the time evolution of a sinusoidally driven pendulum. It has been extensively studied by Chirikov,[7] Greene,[8] Shenker and Kadanoff,[9] Mackay,[10] and many others.[11] We will discuss this map in Appendix B. We note here that from a dynamical systems point of view, *all* the solutions of Eqs. (1.3) or (1.4) are important, but the existence of a Hamiltonian in our case selects out a special set of states which are the ground states. Since it is hard to make general statements about the dynamical system in the large-V regime where most of the states are chaotic, the standard map has been investigated primarily in the small-V regime. In our case, the condition that solutions of Eq. (1.3) be ground states enables one to make physical interpretations of the behavior of the system of balls for all values of the potential, thus interpreting previous results for weak potentials and extending them into the strong potential regime. In spite of claims in the literature to the contrary,[12] the states corresponding to chaotic solutions of the time evolution in Eq. (1.4) are *never* ground states of the system. This brings us to the definition of ground states.

The natural spacing a enters the potential energy in Eq. (1.1) only as a pressure (or chemical potential) term $P=-Ka$ which couples only to the density or the *average* particle spacing and does not enter the equilibrium conditions in Eqs. (1.2). We first consider the absolute ground states with a given pressure, i.e., those states with the lowest possible energy per particle. These states will have a definite average relative periodicity

$$\alpha=\lim_{j\to\infty}\frac{1}{bj}(Z_j-Z_0) \quad (1.5a)$$

$$=\lim_{j\to\infty}\frac{1}{2\pi j}(X_j-X_0) \ , \quad (1.5b)$$

measured in units of the wavelength b of the potential. Aubry[6] has proven that for each α, there exists a pressure P whose corresponding ground state has periodicity α; i.e., α is a continuous function of P.

If α is a given rational, there is a finite range of pressures that gives a ground state with periodicity α, but an irrational α corresponds to a unique pressure. For small values of the potential V, if P is varied smoothly, α will be irrational a finite fraction of the time. However, for sufficiently large V, it is believed that[1,6(a),6(c),6(f),6(i)] the set of P for which α is irrational has measure zero. Despite this, the periodicity can always be fixed at an irrational value by boundary conditions, pressure, or by fixing the total number of balls in a given large region.

In this paper we will consider states with a value of α fixed by the boundary conditions. The ground state of an infinite system with a given value of α can be obtained as the limit of the absolute energy minima of finite-size systems with N balls with the pressure chosen so that the average relative periodicity of the ground states is α in the limit $N\to\infty$.[6(c),23] The ground states with relative periodicity α can also be obtained by considering a periodic infinite system whose energy cannot be lowered by moving a finite number of balls. Aubry[6] has proven that the ground states of the system with average relative periodicity α are in fact periodic. The position of the jth ball in any ground state (which can be degenerate by an overall phase; see Sec. II) is given by

$$X_j=2\pi\alpha j+g(2\pi\alpha j) \ , \quad (1.6)$$

where g is periodic with period 2π (the period of the substrate).

The nature of the ground states depends sensitively on the relative periodicity α. If α is rational, then the system is commensurate and the problem is relatively simple since there is only a finite collection of nonequivalent balls. For this case a well-behaved convergent perturbation theory for small V can be constructed. Translational invariance is broken for all V, and no zero-frequency phonon mode exists. However, when α is irrational the system is incommensurate and the situation is more complicated. The perturbation expansion for small V suffers from "small denominators," so its convergence is problematical.[13] Aubry[6] has shown that if α is a "good" irrational (see Appendix A), then for sufficiently small V a zero-frequency mode exists, but as V increases the zero-frequency mode disappears. However, it is believed that for any V, pinned incommensurate ground states occur for a set of α_0 with zero measure.[6(a)]

In this paper we hope to gain some insight into the nature of the incommensurate states, and in particular, we wish to study critical behavior near the disappearance of the zero-frequency mode for a given α. In Sec. II, which is primarily didactic, we relate pinning to properties of the phonon spectrum, review the continuum approximation and perturbation theory for Eq. (1.2), and demonstrate the existence of a pinned state for large V. In Sec. III we define a disorder parameter and correlation function and also describe the numerical calculations. Section IV consists of results that demonstrate scaling behavior of the disorder parameter and correlation length, while Sec. V contains speculations and conclusions. Appendix A is a summary of basic results of the number theory of irrational numbers relevant to the calculations, and in Appendix B we relate our results to previous work on dynamical systems.

II. PINNED AND UNPINNED PHASES

A. Relation of pinning to the phonon spectrum

In this section we show that the absence of a zero-frequency phonon mode implies the existence of a pinned state for a small applied force. Given a physically stable solution $\{X_j\}$ to the force equations

$$X_{j+1}-2X_j+X_{j-1}-V\sin X_j=0 \ , \quad (2.1)$$

we wish to know whether a nearby solution $\{X_j'\}$ exists with a small uniform force F added

$$X'_{j+1}-2X'_j+X'_{j-1}-V\sin X'_j+F=0 \ . \tag{2.2}$$

By "nearby" we mean that $\delta X_j = X'_j - X_j$ approaches zero as $F\to 0$. If a solution exists, then the system is pinned; i.e., the balls will only move a finite amount when a small force is applied. Expanding (2.2) for small δX_j and assuming that the expansion is well behaved, we find that a solution exists for small F if the equations

$$\delta X_{j+1}-(2+V\cos X_j)\delta X_j+\delta X_{j-1}=-F \tag{2.3}$$

have a solution.

We now consider the phonon spectrum of the same set of balls. We assume that the equations of motion are obtained from a Hamiltonian formed by adding a kinetic energy term to Eq. (1.1) with the mass chosen to scale out of the equations of motion. Given the same $\{X_j\}$ from Eq. (2.1), the linearized equations of motion for small displacements U_j are

$$\frac{d^2U_j}{dt^2}=U_{j+1}-(2+V\cos X_j)U_j+U_{j-1} \ . \tag{2.4}$$

Equations (2.3) and (2.4) are extremely similar. Both can be written in terms of the dynamical matrix

$$M_{ij}=(2+V\cos X_j)\delta_{ij}-\delta_{ij-1}-\delta_{ij+1} \tag{2.5}$$

as

$$\overleftrightarrow{\mathrm{M}}\cdot\delta\vec{\mathrm{X}}=F\vec{a} \quad \text{where } \vec{a}^{\,T}=(1,1,\ldots,1) \ , \tag{2.6}$$

and

$$\frac{d^2\vec{\mathrm{U}}}{dt^2}=-\overleftrightarrow{\mathrm{M}}\cdot\vec{\mathrm{U}} \ , \tag{2.7}$$

respectively.

Stability of the solution $\{X_j\}$ of Eq. (2.1) implies that all the eigenvalues of $\overleftrightarrow{\mathrm{M}}$, which are the squares of the phonon frequencies, are non-negative. If all the eigenvalues are strictly positive, there is no zero-frequency phonon, and Eq. (2.6) can be solved by inverting $\overleftrightarrow{\mathrm{M}}$. The state is hence pinned. If a zero-frequency phonon exists, $\overleftrightarrow{\mathrm{M}}$ is not invertible. Physically, it appears clear that the zero-frequency phonon, if one exists, will have an eigenvector with all its elements having the same sign, i.e., all the balls moving in the same direction. In this case the vector $\vec{a}$ will not be orthogonal to this eigenvector and hence there will be no solution to Eq. (2.6) and the balls will not be pinned.

Note that in principle there could be a pinned solution with the displacement of the zero-frequency phonon proportional to $F^{1/2}$, for example, rather than F. Arguments based on the effective translational invariance of the system with a zero-frequency phonon and numerical work both strongly suggest that this does not happen.[14] We have also ignored potential subtleties of the limit of an infinite number of balls; however, these should not affect the result that the lack of pinning and the existence of a zero-frequency mode are equivalent.

B. Continuum approximation, solitons, and discommensurations

Frank and Van der Merwe[5] studied static solutions of the continuum approximation to Eq. (2.1)

$$\frac{d^2x}{dj^2}=V\sin x \ . \tag{2.8}$$

Naively, this approximation is valid when $X_{j+1}-2X_j+X_{j-1}$ is much less than (X_j-X_{j-1}), i.e., the scale of the change in variation of X is much less than the average separation between the balls. (Note that in this section j is considered to be a continuous variable.)

This equation is the famous sine-Gordon equation, which exhibits soliton solutions (see Fig. 1). These solitons have been described in enormous detail[15] and we note here only that the solitons are unpinned; in other words, the continuum system has a zero-frequency mode. This is proved by examining the equation of motion in the continuum approximation,

$$\frac{\partial^2 x}{\partial t^2}=\frac{\partial^2 x}{\partial j^2}-V\sin x \ . \tag{2.9}$$

The linearized equation of motion for a small distortion δx about a stationary solution x_0 is

$$\frac{\partial^2}{\partial t^2}\delta x=\frac{\partial^2}{\partial j^2}\delta x - V\,\delta x\cos x_0 \ . \tag{2.10}$$

It is straightforward to show that

$$\delta x=\left.\frac{\partial x}{\partial j}\right|_{x_0} .$$

is a zero-frequency eigenmode of this equation.

In a weak potential an incommensurate system which is nearly commensurate (i.e., one whose relative periodicity is close to a rational with a small denominator) can be thought of as consisting of almost commensurate regions (domains) separated by regularly spaced domain walls or discommensurations—which in the continuum limit are just the solitons of the sine-Gordon equation. It is instructive to consider the motion of a single wall that is well separated from others. The zero-frequency mode discussed above exists because, in this continuum limit, one

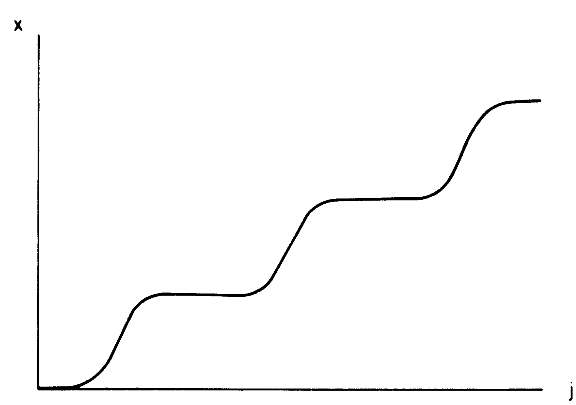

FIG. 1. Solution to the (continuous) sine-Gordon equation, exhibiting solitons.

soliton can be moved an infinitesimal amount by moving each of the balls (here a continuum of balls) an infinitesimal amount. In the discrete case (which is the case of interest to us), as the domain wall moves, some of the balls must move from one valley of the potential to another by going over the maxima in the potential. This can only be accomplished in a continuous way, if, at any position of the wall, there are balls arbitrarily close to the top (i.e., maximum) of the potential. If this is *not* the case, in order for the wall to be moved to a position with the *same* energy, it must be moved by a *discrete* amount and at least one ball must jump from one side of a maximum of the potential to the other. Since this cannot be accomplished with small displacements, the wall is pinned and there is no zero-frequency mode. This is due to the breakdown of the continuum approximation: In a sense (to be made precise later) x_0 is no longer a continuous function of j and $\partial x_0/\partial j$ no longer exists. An extension of this argument from an almost commensurate system to the general discrete incommensurate case suggests that a state will be unpinned if and only if there are balls in the ground state arbitrarily close to the top of the potential. This idea forms the basis for the definition of a disorder parameter in Sec. III and for many of the physical arguments in this paper.

Estimates of the discommensuration pinning energy, the energy barrier which must be overcome to move a domain wall in an almost commensurate system, have been made by several authors[16]; generally they calculate the wall shape using the continuum approximation and evaluate the resulting dependence of the energy on the location of the discommensuration. For an almost commensurate system the continuum approximation will be valid only for extremely small potential strengths; however, in this limit, the domain walls will be so broad that their definition is murky. Thus, if there are a small number of balls per period of the potential, a description of the system in terms of continuum solitons is probably *never* valid, in spite of its prevalence in the literature. However, Joos[17] has found that the qualitative behavior of the pinning energy as a function of V is reproduced by this approximation.

C. Perturbation theory and the unpinned state

One can glean a great deal of insight about the system by carefully examining the weak substrate potential perturbation theory for both commensurate and incommensurate phases. The expansion parameter is simply V. As made clear by Kolmogorov,[13] it is important to do the perturbation expansion at *fixed* relative periodicity α.

The force equations for a system with substrate wave vector $q=2\pi\alpha$ measured in units of the average ball spacing, can be written in the form

$$f_j=Y_{j+1}-2Y_j+Y_{j-1}-V\sin(qj+Y_j)\ . \tag{2.11}$$

Here $Y_j=X_j-qj$ is defined so that $Y_j=0$ is a ground state of the system when $V=0$.

We first consider the stationary states of the system, the solutions to $f_j=0$, which we denote by $Y_j=\bar{\delta}_j$, where

$$\bar{\delta}_{j+1}-2\bar{\delta}_j+\bar{\delta}_{j-1}-V\sin(qj+\bar{\delta}_j)=0\ . \tag{2.12}$$

For $V\ll 1$ we would like to expand the sine in a Taylor series, assuming $\bar{\delta}_j$ is $O(V)$. However, at this point one must be careful and allow for a uniform phase shift, i.e., a preferred overall position of the balls relative to the substrate. We hence write

$$\bar{\delta}_j=\Delta_0+\delta_j\ ,$$

where now $\delta_j=O(V)$, and thus

$$\delta_{j+1}-2\delta_j+\delta_{j-1}-V\sin(qj+\Delta_0+\delta_j)=0 \tag{2.13}$$

which to lowest order in V gives

$$\delta_j^{(1)}=-\frac{V}{2(1-\cos q)}\sin(qj+\Delta_0)\ . \tag{2.14}$$

This solution is uniformly small unless $\cos q$ is very close to 1, i.e., q is near 2π. If q exactly equals 2π (i.e., lowest-order commensurate) then the divergence can be eliminated by adjusting Δ_0 to be either 0 or π, which makes $\delta_j^{(1)}$ identically zero. The balls are thus in this case "locked" onto the substrate, but the perturbation theory is perfectly well behaved. On the other hand, if q is near to but not exactly 2π [i.e., $(2\pi-q)^2\lesssim V$] the divergence is not eliminated by adjusting Δ_0 and the perturbation theory is useless, due to the small denominator; Pokrovsky[16] calls this the first "dangerous zone" in q.

If the lowest-order correction to Y_j is not too large, the next step is to plug $\delta_j^{(1)}$ back into Eq. (2.13) to find the second-order contribution. When this is done, one finds $\delta_j=\delta_j^{(1)}+\delta_j^{(2)}$, where

$$\delta_j^{(2)}=\frac{V^2}{8(1-\cos q)(1-\cos 2q)}\sin[2(qj+\Delta_0)]\ . \tag{2.15}$$

This expression is troublesome near $q=2\pi$ (which has already been excluded) and also at $q\cong\pi$. When $q=\pi$, one can adjust Δ_0 to be 0 or $\pi/2$ (or, equivalently, π or $3\pi/2$), again locking the balls to the substrate, but, as before, if q is near but not equal to π, the perturbation theory is badly behaved.

This procedure can clearly be continued. At nth order, one finds that a new dangerous zone of width (in q) of $O((\sqrt{V})^n)$ appears corresponding to a new harmonic of q. If q is not exactly commensurate but is in the dangerous zone, the perturbation theory is divergent, but if nq exactly equals an integral multiple of 2π, then by adjusting Δ_0 the divergence can be eliminated at the price of locking the balls onto the substrate.

One should note, however, that for the *commensurate* case, where at some order, $nq/2\pi$ is integral, two inequivalent choices of Δ_0 always exist when the balls lock. One corresponds to a minimum and the other to a saddle point of the energy. We are primarily concerned here with the energy minimum, which is the ground state with the rational periodicity $\alpha=q/2\pi$. The other state is the lowest saddle point of the energy (about which there is one unstable direction), which we will call the "saddle state." We have examined 8 orders in perturbation theory and have found that the stable solution does not have a ball sitting at the top of a well, while the saddle state does. Greene[8] has observed this result for *small* V and, in addition, that in both the solutions all the balls are symmetrically placed about either $X=0$ or π. One can see this in a physical way as follows: If there are an odd number of balls in the unit cell, then putting two balls equidistant from the top allows them to more efficiently minimize their potential energy (we have used the reflection symmetry); see Fig. 2(a). When the number of balls is even, at first it is not clear which state in Fig. 2(b) is preferable—the one with balls in the bottoms and the tops or the other symmetric state. However, if one considers the energy of spring stretching, one finds that is necessary to stretch more springs to let the balls in the former solution "settle in," so it appears to have higher energy.

On the basis of these considerations, we expect that for *all* V the stable ground-state solution for a commensurate system will never have a ball at the top of a well and will always have the balls symmetrically placed about $X=0$ or π. Hence any commensurate system will have *no* zero-frequency phonon and will be pinned for any value of the potential. This can easily be verified in perturbation theory: If the balls lock at nth order, a gap to the lowest-frequency phonon will appear at the same order in perturbation theory.

For an *incommensurate* system with α irrational, it is not clear whether the perturbation theory converges. Eventually one reaches an order n where for some m, $|qn-2\pi m|<\epsilon$ for any ϵ, but, intuitively, if n is large enough then the large denominator will be compensated by the small factor V^n. This situation is precisely the one addressed by the Kolmogorov-Arnol'd-Moser[13] (KAM) theorem. The theorem implies that at fixed α, if α is far enough from every rational (see Appendix A) and V is small enough, then the factors of V^n do indeed wash out the small denominators and the perturbation theory converges. Only if the $|qn-2\pi m|$ are not bounded below by a negative power of n does the perturbation theory have a vanishing regime of validity.

In the regime where the perturbation theory converges for a given α which is sufficiently irrational (see Appendix A), Aubry[6] has shown that a zero-frequency phonon mode exists. The proof is analogous to the proof for the continuum approximation. In the incommensurate discrete case, the zero-frequency phonon eigenvector $\{U_j\}$ must satisfy

$$U_{j+1}-2U_j+U_{j-1}-U_jV\cos(qj+\Delta_0+\delta_j)=0\ , \tag{2.16}$$

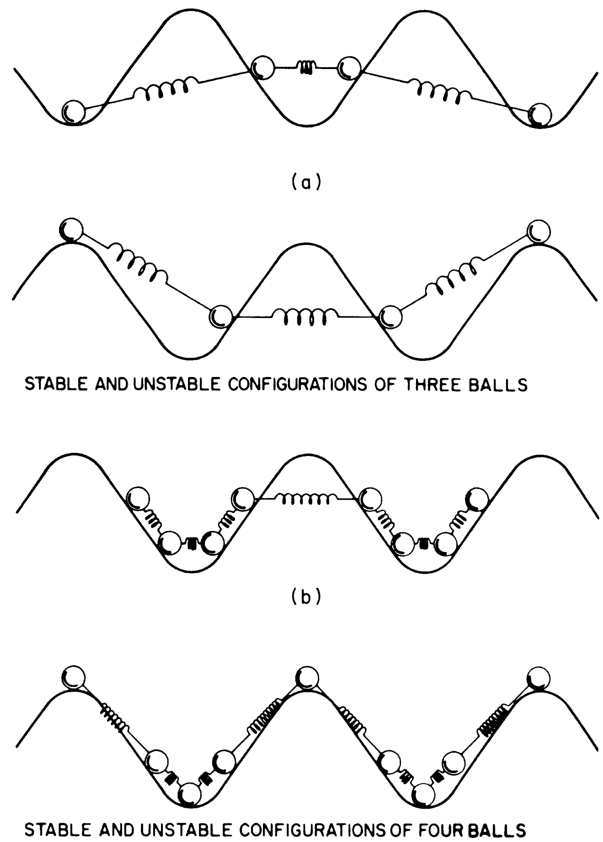

FIG. 2. (a) Stable and unstable configurations of three balls (typical of an odd number of balls). (b) Stable and unstable configurations of four balls (typical of an even number of balls). In both cases, the stable configuration does not have a ball at the top of a well.

where we have expanded about the stable solution by setting $Y_j=\delta_j+\Delta_0+U_j$. As Aubry points out, the KAM theorem implies that δ_j is an analytic function g of $qj+\Delta_0$ where Δ_0 is an *arbitrary* phase which determines the overall position of the balls. Therefore it is well defined to set

$$U_j=1+\frac{dg}{d(qj+\Delta_0)}\ . \tag{2.17}$$

This distortion is the mode we seek, since

$$U_{j+1}-2U_j+U_{j-1}-U_jV\cos(qj+\Delta_0+\delta_j)=\frac{d}{d(qj+\Delta_0)}[\delta_{j+1}-2\delta_j+\delta_{j-1}-V\sin(qj+\Delta_0+\delta_j)]=0\ . \tag{2.18}$$

Thus the existence of a KAM trajectory implies that the threshold force to make the balls slide is 0. When the perturbation theory is divergent, on the other hand, $d\delta_j/d(qj+\Delta_0)$ no longer exists and the proof breaks down. Note that in contrast to commensurate states for which the overall phase Δ_0 can take only discrete values (signifying locking to the substrate), Δ_0 is arbitrary for incommensurate states, corresponding to translational invariance.

D. Existence of the pinned state

One of Aubry's major contributions is his proof that for sufficiently large V the ground state is pinned even in the incommensurate system. One can see this result intuitively by considering the limit $V \to \infty$, where it is clear that the balls lie in the bottoms of the potential wells. If one tries to move the balls an infinitesimal amount, they do not slide smoothly but are stuck in the concave potential wells. Although it is true that one could have constructed a state degenerate in energy which is near to the original one, in order to reach it a ball must "jump over" a finite barrier, so there is no continuous motion that leaves the energy invariant. By this argument, one can also see that the existence of metastable states is closely connected with pinning, since the system cannot smoothly iron out defects in its structure if metastable states exist.

Aubry[6] has proved many results about the nature of the ground states of the system with relative periodicity α equivalent to a relative substrate wave vector $q = 2\pi\alpha$. The result of Aubry that we use most heavily is that the position of the jth ball can be written, for any V, as

$$X_j = qj + \Delta_0 + g(qj + \Delta_0) , \tag{2.19}$$

where Δ_0 is an arbitrary constant phase, and g is odd, bounded by $\pm\pi$, and periodic with the substrate period 2π. Aubry calls $g(qj+\Delta_0)$ the *hull function* of the ground state. A physical picture of the hull function is obtained by considering a system with a continuously variable V. When V is zero, the position of the jth ball is $qj+\Delta_0$, where Δ_0 is an arbitrary phase that reflects the translational invariance of the system. If V is adiabatically increased from zero keeping the average spacing of the balls fixed, the balls fall down into the wells. The hull function determines where the jth ball is located when V is finite; its existence implies that X_j is a function only of where the jth ball was when V was zero. The bounds on g imply that each ball will fall into the closest well (without hopping over a barrier). The state so obtained will be the ground state with the original periodicity. Aubry further showed (as mentioned above) that $g(qj+\Delta_0)$ is analytic for sufficiently small V, and conversely that when the balls are pinned the hull function becomes discontinuous. In fact, he proved that in the pinned phase $X_j(qj+\Delta_0)$ is the sum of a countable number of Heaviside step functions and the balls hence lie only at a countable set of values of the local potential. It follows that the expression (2.17) for the zero-frequency mode in perturbation theory is identically zero whenever it exists and hence is not an eigenmode, verifying that in the pinned phase no zero-frequency mode exists. We provide simple arguments below which show that the pinned phase must exist for sufficiently large V without relying on theorems about the hull function.

We first show that the *existence* of a hull function implies that for sufficiently large V, each ball sits in the bottom half of a well (i.e., such that $-V\cos X_j < 0$). (Aubry has proved this result also, but the argument here is simpler, though only rigorous for finite-size systems.) The existence of a hull function is invoked here only to put a bound on the distance between successive balls, so the arguments can be trivially generalized to show that metastable states with bounded ball separations are also pinned.

First we note that stability of the system to small perturbations of the ball positions implies that

$$0 \le \frac{\partial^2 U}{\partial X_j^2} = 2 + V\cos X_j . \tag{2.20}$$

This condition is necessary but not sufficient for stability; it merely says that any small motion of one ball cannot lower the system's energy. From Eq. (2.20) the condition

$$\cos X_j \ge -2/V \tag{2.21}$$

must hold, which implies that the balls cannot be at the tops of the wells for large V. Since the hull function g is bounded by $\pm\pi$, the maximum spring force on the jth ball in the ground state is less than 4π. The magnitude of the force from the potential is $V\,|\sin X_j\,|$, so X_j must satisfy

$$|\sin X_j\,| \le 4\pi/V , \tag{2.22}$$

which implies

$$|\cos X_j\,| \ge [1-(4\pi/V)^2]^{1/2} . \tag{2.23}$$

If $V \ge 2(1+4\pi^2)^{1/2}$, then the only way to satisfy both (2.21) and (2.23) is for $\cos X_j$ to be positive for all j. Thus, the balls must all be in the bottom halves of the wells for sufficiently large V.

Aubry then proved that if each ball is in the lower half of a well, no zero-frequency mode exists. This can again be easily demonstrated by a simple physical argument. As shown previously, the balls are pinned to the wells if the matrix $\overleftrightarrow{M}$ defined in Sec. II A is positive definite. Since, as shown above, for large V, $V\cos X_j > 0$ for all j, $\overleftrightarrow{M}$ can be written as a sum of two matrices $\overleftrightarrow{A}$ and $\overleftrightarrow{B}$, with

$$A_{ij} = 2\delta_{ij} - \delta_{i,j+1} - \delta_{i,j-1} ,$$
$$B_{ij} = \delta_{ij} V\cos X_j ,$$

where $\overleftrightarrow{B}$ is positive definite. Equation (2.23) implies that each eigenvalue of $\overleftrightarrow{B}$ can be made bigger than any arbitrary Λ_0 by making V sufficiently large. The eigenvalues of $\overleftrightarrow{A}$ are of the form $\lambda = 2(1-\cos k)$ and are hence nonnegative, so $\overleftrightarrow{A}$ is positive semidefinite. Since $\vec{v}\cdot\overleftrightarrow{M}\cdot\vec{v} = \vec{v}\cdot(\overleftrightarrow{A}+\overleftrightarrow{B})\cdot\vec{v} \ge 0 + \Lambda_0$ for any normalized vector $\vec{v}$, it follows that the eigenvalues of $\overleftrightarrow{M}$ are bounded below by Λ_0, and hence, even in the infinite system no zero-frequency mode of the balls exists and the system is pinned. Aubry has actually proven stronger results than those quoted here, but the simple arguments presented in this section are sufficient to demonstrate that a transition must occur between pinned and unpinned phases in an incommensurate system.

III. DISORDER PARAMETER, CORRELATION FUNCTION, AND RATIONAL APPROXIMATION

We are interested in studying the behavior of incommensurate systems near the critical value $V_c(\alpha)$ of the potential which separates the unpinned from the pinned phase for a given relative periodicity α. In order to make analogies with usual critical phenomena, it is useful to consider one of the two phases as ordered and the other as disordered. Since there is no broken symmetry in the conventional sense in either phase, this identification is not at all clear. However, the unpinned phase does have several features which are characteristic of conventional ordered phases: It has a zero-frequency (Goldstone) mode and has correlations which extend to arbitrarily long distances (in a sense which we will make more precise later). However, there is no obvious order parameter, and it is thus simpler to define a *disorder parameter* that is zero only in an infinite incommensurate unpinned system. Motivated by the belief that the unpinned and pinned phases are distinguished by whether or not there are balls arbitrarily close to the tops of wells in the physically stable solution, we define the "disorder" parameter by

$$\psi = \min_{j,n} |X_j - 2\pi(n+\tfrac{1}{2})| \ , \tag{3.1}$$

which is just the minimum distance (measured along the x axis) of any ball from the top of a well. As long as ψ is finite, the balls are pinned, and $\psi=0$ corresponds to the unpinned phase. Note that this disorder parameter is not an average—as seen previously, the average distance from the top can be quite large in the continuum model, even though the solution is unpinned. For any finite system, and similarly for any commensurate system, ψ will always be nonzero.

In order to numerically study the properties of an incommensurate system with periodicity α, we use a method originally due to Greene[8] and study a sequence of commensurate systems with rational periodicities Q_n/P_n which approximate the incommensurate system.[18] The natural and most rapidly converging sequence of rational approximations is given by the continued fraction expansion of α (see Appendix A). For definiteness, we study the golden mean $\phi=(1+\sqrt{5})/2$ whose continued fraction is just $[1,1,1,1,1,\ldots]$. The sequence $\{Q_n/P_n\}$ of rational approximants (which in this case are ratios of successive Fibonacci numbers) converges more slowly for ϕ than the sequence for any other number; in this sense it is the most irrational of all irrational numbers. A system with relative periodicity $\alpha=\phi$ thus has the advantage of being least likely to be affected by being close to a low-order rational number, i.e., the system is unlikely to show "almost commensurate" behavior.

In addition, as for all other quadratic irrationals [those of the form $(a+b\sqrt{n})/c$ with a, b, n, and c integers], the continued fraction of ϕ is periodic and hence the system of balls might be expected to show the simplest scaling behavior near the critical value of V. In Sec. V we make some conjectures about extensions of our results to other irrational periodicities.

Since commensurate systems are equivalent to finite-size systems with periodic boundary conditions, computations on a commensurate system with periodicity Q_n/P_n can be performed by finding solutions to P_n force equations (with periodic boundary conditions) of the P_n balls in Q_n periods of the potential. Two solutions are found, one corresponding to the minimum of the energy and the other the lowest-energy saddle-point solution, which has one ball constrained by symmetry to be at the top of a well.

It is clear from the discussion in Sec. II C that the ground state and the saddle state should have axes of reflection symmetry; this has been checked numerically. If P_n is odd, one expects the ground state to have a ball in the bottom of a well, and if P_n is even, one expects it to have two balls symmetrically placed about the bottom of a well. In the limit of $Q_n\rightarrow\infty$ the minimum energy solution approaches the ground state of the system with periodicity $\alpha=\phi$. The saddle solution is found by fixing one ball at the top of a well and letting the others adjust to minimize their energy subject to this constraint. We shall see that for $V<V_c$, this solution also approaches the incommensurate ground state as $Q_n\rightarrow\infty$, but for $V>V_c$ the incommensurate saddle solution is *distinct* from the ground state. In order to reliably obtain the desired solutions, we explicitly impose symmetry on the solutions and solve the $P_n/2$ [or $(P_n-1)/2$] force equations for each V and then slowly increase V.

This method is quite different from that used in Refs. 7–11. In those calculations, after using symmetry to eliminate X_0 as a variable, the Eqs. (2.1) were used to obtain X_{P_n} as a function of X_1 and the solution determined by requiring $X_{P_n}-X_0=2\pi Q_n$. Our method has the disadvantage of requiring the solution of many simultaneous force equations, but it enables us to study the pinned regime $V>V_c$ which is inaccessible by the dynamical systems methods of Refs. 7–11.

Two calculations were performed. In the first, the ground state was found numerically and the distance of the balls from the tops of the wells calculated. One can think of this calculation as measuring correlations of the balls with the substrate potential; the minimum distance is just the disorder parameter. The second calculation involved comparing the ground-state and lowest saddle-point solutions. This was done by starting with the ball at the top of a well in the saddle-point solution and one of the two balls closest to the top in the ground-state solution and calculating their spatial separation, with the origin chosen to be at the maximum (or the nearest maximum) of the potential. The two solutions were then compared by labeling these balls "0" and then calculating the separation $\Gamma(j)$ between the jth balls in the two solutions. This procedure measures correlations of the two solutions with each other. The easiest way to gain insight into the behavior of this separation as a function of j is to consider the $V=0$ and ∞ limits. (Using renormalization-group arguments, we expect qualitative features of the unpinned region to be determined by the $V\rightarrow 0$ behavior and those of the pinned region to be determined by the $V\rightarrow\infty$ behavior.) When $V=0$, for a commensurate system with P balls in Q wells, the two solutions maintain a constant separation of $2\pi/2P$. On the other hand, when $V\rightarrow\infty$, the zeroth balls in the two solutions are separated by π, but every succeeding difference is 0. Thus, intuitively one expects that in the small-V unpinned phase the two solutions stay distinct for all j, while in the large-V pinned phase, far from the ball 0 which is locked at the top in the saddle-point solution, the ground state and saddle state are basically indistinguishable.

IV. RESULTS AND SCALING

Since ψ is nonzero for any finite or commensurate system, we expect the system size or the number of balls per unit cell to be analogous to finite size in a spin system.

We thus expect a scaling behavior for ψ as a function of V and P_n for n large and $V \sim V_c$ of the form

$$\psi(V,P_n) \sim |\epsilon|^{\sigma} f(\epsilon P_n^{1/\bar{\nu}}) , \tag{4.1}$$

where $\epsilon = V - V_c$. The scaling function f should have various limits which can be determined. In particular, for any finite P_n, one expects finite-size effects to dominate when ϵ is so small that $\epsilon P_n^{1/\bar{\nu}}$ approaches zero. Hence $f(y) \sim 1/|y|^{\sigma}$ for $y \to 0$ and

$$\psi(V_c,P_n) \sim \left| \frac{1}{P_n} \right|^{\sigma/\bar{\nu}} . \tag{4.2}$$

The function $\tilde{f}(y) = |y|^{\sigma} f(y)$ is thus expected to be smooth at $y = 0$.

In the opposite limit, for *fixed* (nonzero) ϵ, the limit $P_n \to \infty$ yields results for the incommensurate system which should be independent of P_n provided $P_n \gg \epsilon^{\nu}$. Thus on the pinned side $f(y)$ approaches a constant as $y \to +\infty$ and hence

$$\psi(V,P_n = \infty) \sim |\epsilon|^{\sigma} \tag{4.3}$$

for $V > V_c$. The exponent σ is thus the disorder parameter exponent. On the unpinned side we expect $\lim_{y \to -\infty} f(y) = 0$, but it is useful to ask how $f(y)$ tends to zero as $y \to -\infty$. To do this we consider turning on the potential adiabatically from a $V = 0$ state which has the symmetry of the ground state for $V > 0$, i.e., with a ball at $X = 0$ for P_n odd or balls symmetrically placed about $X = 0$ for P_n even. The closest ball to the top of a well in each of these cases is a distance $2\pi/2P_n$ from the top at $V = 0$. This ball will also be the closest to the top at $V > 0$ and hence will determine $\psi(V,P_n)$. In the limit $P_n \to \infty$, the function which yields the positions of the balls in the ground state as a function of their positions at $V = 0$ should approach the function for the incommensurate case; the position of a ball x, initially at x_0, will be $x = x_0 + g(x_0)$ where g is the hull function defined in Sec. II D. Hence we can conclude that as $n \to \infty$

$$\psi(V,P_n) + \pi \to \pi + \frac{2\pi}{2P_n} + g\left[\pi + \frac{2\pi}{2P_n}\right] . \tag{4.4}$$

However, by reflection symmetry, as long as $V < V_c$, $g(\pi) = 0$ (g is odd about π); thus

$$\psi(V,P_n) \approx \frac{2\pi}{2P_n} + \left[g\left[\pi + \frac{2\pi}{2P_n}\right] - g(\pi) \right] . \tag{4.5}$$

For $V < V_c$, g is analytic and we therefore have

$$\lim_{n \to \infty} \frac{\psi(V,P_n)}{2\pi/2P_n} = 1 + \left. \frac{dg(x_0)}{dx_0} \right|_{x_0 = \pi}$$
$$\equiv \Upsilon(V) . \tag{4.6}$$

The scaling form of ψ implies $f(y) \sim (-y)^{-\bar{\nu}}$ as $y \to -\infty$ and $\Upsilon(V) \sim |\epsilon|^{\sigma - \bar{\nu}}$ as $V \to V_c^-$.

Excellent fit to the scaling form of Eq. (4.1) has been found from a study of the standard map for $V < V_c$ by Shenker and Kadanoff.[9] They find $\sigma/\bar{\nu} = 0.721 \pm 0.001$, $\bar{\nu} = 1.00 \pm 0.015$, and $V_c = 0.971\,635$. Our results, though not as accurate due to the smaller system size, extend the calculations into the pinned regime which is not accessible by the methods of Ref. 9. The disorder parameter data for various values of V are plotted in Fig. 3 as a function of $1/P_n$ for commensurate approximations to the golden mean. On both sides of the pinning transition, the data fit the scaling form of Eq. (5.1) with the exponents quoted above, as shown in Fig. 4.

From the analogies with finite-size scaling in usual critical phenomena, one expects that the exponent $\bar{\nu}$ describing how finite size effects increase the disorder parameter should be equal to the exponent ν of some diverging correlation length in the true infinite incommensurate system. This is in fact the case and we can identify this correlation length on both sides of the transition.

Before discussing the correlation length, we briefly digress and consider whether there is a "disorder field" which is conjugate to our disorder parameter. Since the disorder parameter is a function of the properties of the balls near the tops of the wells, it is natural to consider a perturbation in the Hamiltonian which affects the balls in this region. The simplest choice which will have an anomalous effect only on the balls near the top is just

$$\delta H = -h \sum_j |\cos(\tfrac{1}{2} X_j)| , \tag{4.7}$$

which has a linear cusp at the top of each well. If a small term of this form could be added to the Hamiltonian, the system could no longer exhibit a zero-frequency mode even for small V since the KAM theorem does not apply unless more than three derivatives of the potential are continuous (this is because the Fourier coefficients of a cusplike potential fall off so slowly that they cannot cancel the small denominators in perturbation theory). Balls will *not* be arbitrarily close to the top if h is positive, and hence ψ

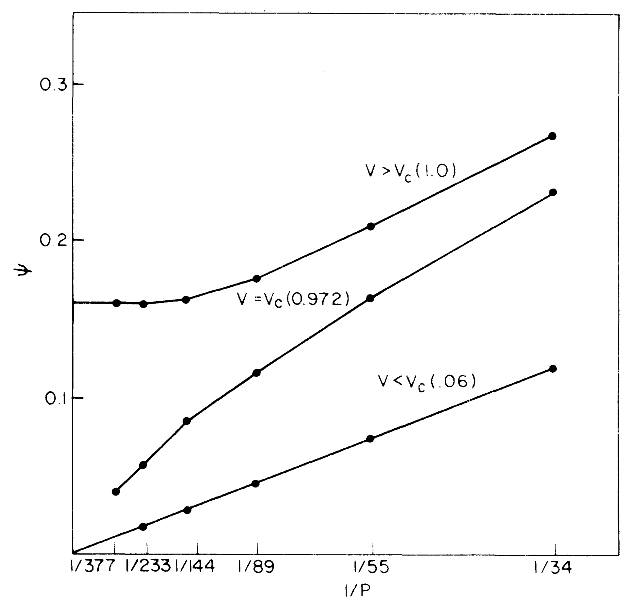

FIG. 3. Behavior of the disorder parameter for three values of V plotted as a function of $1/P_n$. For $V > V_c$ ψ approaches a finite value as $1/P_n \to 0$, but for $V < V_c$ ψ approaches 0 linearly as $1/P_n \to 0$.

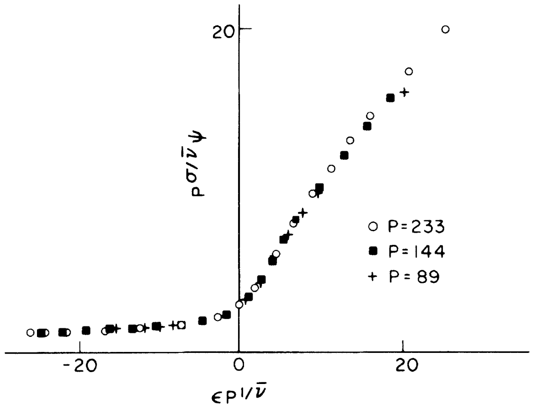

FIG. 4. Scaled disorder parameter $\psi P_n^{\sigma/\bar{\nu}}$ as a function of $\epsilon P^{1/\bar{\nu}}$ ($\epsilon = V - V_c$) for various P with $\bar{\nu} = 1.00, \sigma = 0.721$. The plot is of the scaling function $\tilde{f}(y)$ defined below Eq. (4.2).

will be nonzero and the system will be pinned even for the incommensurate case; presumably there will be no phase transition as a function of V. Unfortunately, it is not at all clear what a physical realization of this disorder field might be.

We now turn to the definition of a correlation length which we define in terms of the differences $\Gamma(j)$ between the ground-state and lowest saddle solutions for finite P_n discussed above. Since the saddle-point solution is obtained by fixing the position of one ball, we can see that the large-j behavior of $\Gamma(j)$ measures the extent of the effects of a forced boundary condition. As discussed above, $\Gamma(j)$ behaves quite differently in the pinned and unpinned phases. We consider the pinned phase first. In Fig. 5, $\Gamma(j)$ is plotted as a function of j for a 377-ball system for various V in this regime.

One can see that for $V > V_c, \Gamma(j)$ falls off as j is increased from its value $\Gamma = \psi$ for $j = 0$ (the boundary conditions at both ends of the system cause the plot to be nearly symmetric about $j = 188$). As $V - V_c$ increases the rate of decay increases. To obtain a length scale characterizing this falloff, the logarithm of $\Gamma(j)$ is plotted versus j; graphs for various values of V are shown in Fig. 6. For $V > 1.0$ an exponential envelope for the falloff is clearly evident, and we define the inverse correlation length $\xi^{-1}(V)$ to be the slope of this exponential. [Since the force equations are solved to one part in 10^8, the values of $\Gamma(j)$ that are less than 10^{-8} exhibit numerical noise and are discarded from the plots.] Close to V_c, the system size becomes comparable to the correlation length and the behavior of $\Gamma(j)$ is not so clear. However, we expect that for values of V for which $1 \ll \xi \lesssim 100$, $\xi(V)$ should behave like $(V - V_c)^{-\nu}$, where ν is the correlation-length exponent of the infinite system. Figure 7 shows a plot of $1/\xi$ as a function of $\epsilon = (V - V_c)$, and it indeed appears that

$$\xi \propto \epsilon^{-\nu}, \tag{4.8}$$

with $\nu = 1.0 \pm 0.04$, and thus, in the pinned region, as expected, $\nu = \bar{\nu}$ (to within the accuracy of our data). In the pinned regime, the behavior of $\Gamma(j)$ for $j \ll P$ appears to approach a well-behaved limit as $P_n \to \infty$, so the informa-

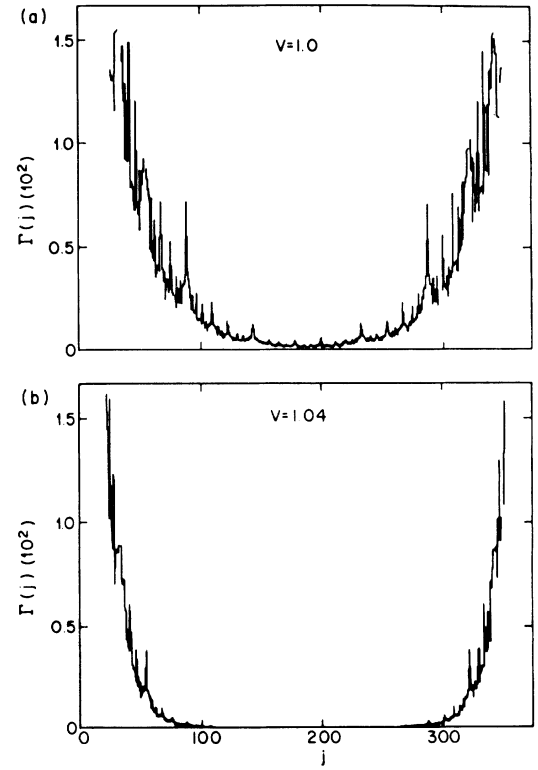

FIG. 5. Difference between stable and saddle solutions $\Gamma(j)$ plotted vs j for two values of $V > V_c = 0.9716$. Note $\Gamma(j)$ decays for j far from the boundaries.

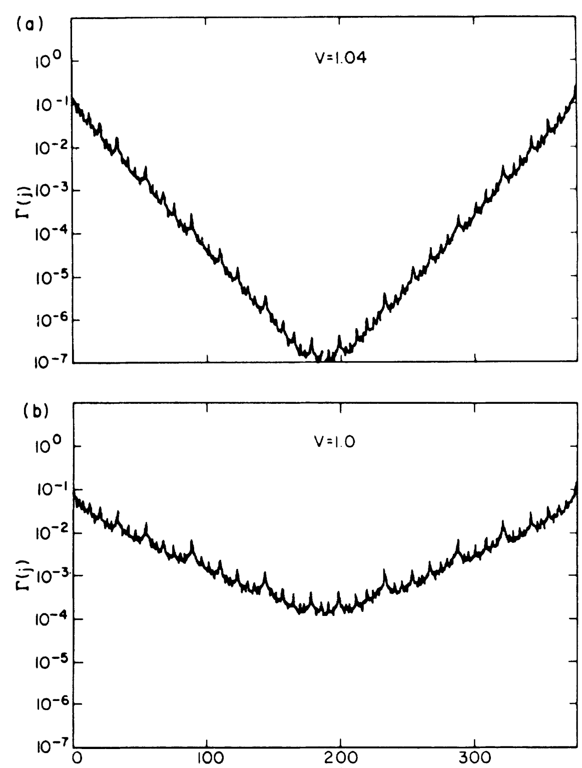

FIG. 6. Semilogarithmic plot of $\Gamma(j)$ vs j for two values of $V > V_c$. The correlation length ξ is defined by fitting the graph's envelope to the form $\Gamma(j) = \psi e^{-j/\xi}$.

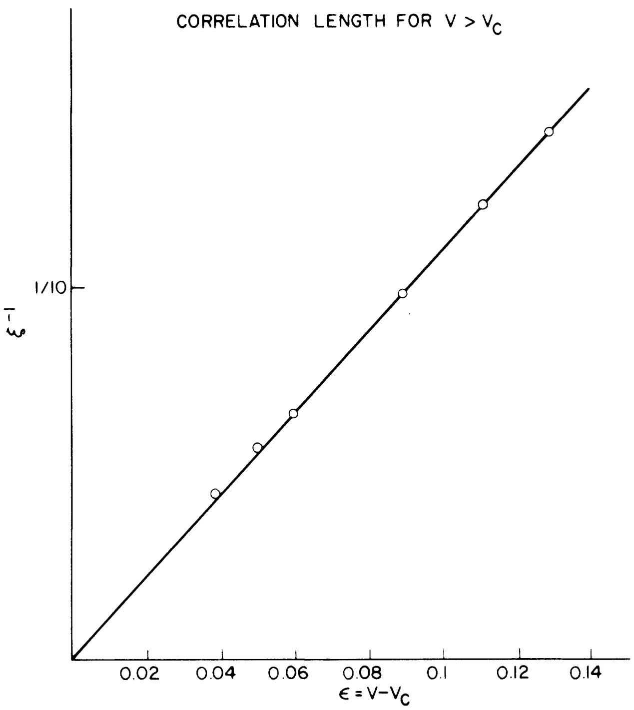

FIG. 7. Plot of inverse correlation length ξ^{-1} vs $V-V_c$, demonstrating that $\xi \propto (V-V_c)^{-\nu}$, with $\nu=1.0\pm0.04$.

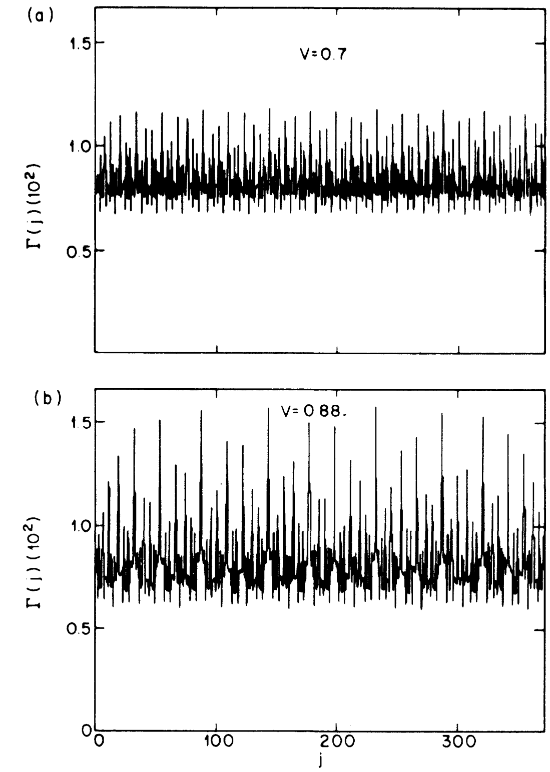

FIG. 8. Difference between the stable and saddle solutions $\Gamma(j)$ plotted vs j for two values of $V<V_c$. $\Gamma(j)$ does not exhibit decay, but has a characteristic length scale of fluctuations.

tion extracted from a system with finite but large P_n should be valid for the true incommensurate system. As in critical phenomena, the correlation length in the disordered phase measures the falloff of the effects of a boundary condition.

In the unpinned region, on the other hand, the behavior of $\Gamma(j)$ is qualitatively different. It is tempting to guess that, by analogy to the spin-spin correlation function in the ordered phase of a magnet, $\Gamma(j)$ will decrease exponentially to a constant value. However, examination of Fig. 8 shows that, for V below V_c, $\Gamma(j)$ has structure that does not decay far from the boundaries. Nonetheless, $\Gamma(j)$ does seem to have a characteristic length scale of variation that increases as V approaches V_c.

We will associate the length scale of the variations of $\Gamma(j)$ with the correlation length in the unpinned phase. Before doing this, we must argue that $\Gamma(j)$ is a sensible quantity to calculate in the unpinned phase even though it approaches zero for each j as P_n approaches infinity. However, for $V<V_c$, $(P_n/\pi)\Gamma_{P_n}(j)$ is just an approximation to the derivative of the hull function $g(X_0)$. This fact can be seen by noting (as above) that $X_0=\pi$ corresponds to the ball at the top in the saddle solution (i.e., the zeroth ball), while $X_0=\pi+2\pi/2P_n$ corresponds to the ball in the ground-state solution that is closest to the top (again $j=0$). Similarly, for general j we have

$$\Gamma_{P_n}(j)\approx g\left[\pi+q_nj+\frac{\pi}{P_n}\right]-g(\pi+q_nj)\ ,$$

where $q_n=2\pi Q_n/P_n$. Since g is analytic for $V<V_c$, the limit as $P_n\to\infty$ of $(P_n/\pi)\Gamma_{P_n}(j)$ is well defined, and is just $1+dg(X_0)/dX_0\,|_{X_0=qj+\pi}$. The hull function $g(qj+\pi)$ is a quasiperiodic function of j, so $\Gamma(j)$ must be quasiperiodic also, which explains why exponential decay is not observed.

Thus for $V<V_c, \Gamma_{P_n}(j)$ goes to zero as P_n gets large, but $P_n\Gamma_{P_n}(j)$ tends to a nonzero value for all j, while for $V>V_c$, $\Gamma(j)$ approaches a limit as $P_n\to\infty$, but it exhibits exponential decay as j increases.

In order to gain more insight into the behavior of $\Gamma(j)$ for $V<V_c$, it is useful to calculate its Fourier transform $\Gamma_P(k)=\sum_j e^{ijk}\Gamma_P(j)$; the corresponding structure factor $I_{377}(k)=|\Gamma_{377}(k)|^2$ is plotted as a function of k in Fig. 9 on a semilogarithmic plot. Note that the values of k allowed by the boundary conditions are multiples of $2\pi/377$. One can see that $I(k)$ falls off for very small k; this fact is directly related to the exponential convergence of the perturbation theory implied by the analyticity of g.

This exponential convergence implies that the contribution of the nth order of perturbation theory (for n large but less than the number of balls in the system) to $\Gamma(j)$ is of order $e^{-\gamma n}$ for some $\gamma>0$. This is because the first nonzero contribution to $\Gamma(nq)$ occurs at nth order in perturbation theory. The wave vector nq is equivalent to some $(nq-2\pi m)$ in the first Brillouin zone (for m an integer). The magnitude of $I(k)$ for k near zero is thus determined (at least for small V) by the value of n necessary for $|nq-2\pi m|$ to be k. As discussed in Appendix A, for quadratic irrationals the minimum such value of n goes as $1/k$, so that as k approaches zero $\Gamma(k)$ should be of order $e^{-\gamma/k}$. Therefore, we expect that a semiloga-

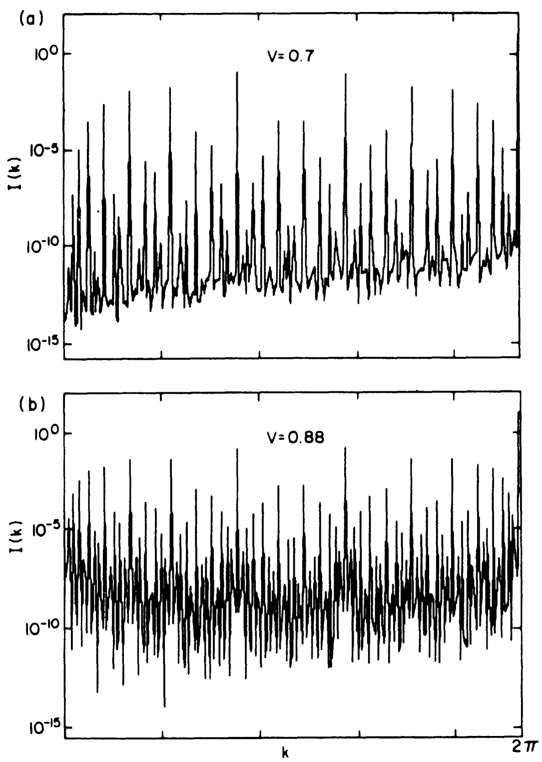

FIG. 9. Plot of structure factor $I(k)=|\sum_j e^{ikj}\Gamma(j)|^2$ vs k on a semilogarithmic scale for two values of $V<V_c$.

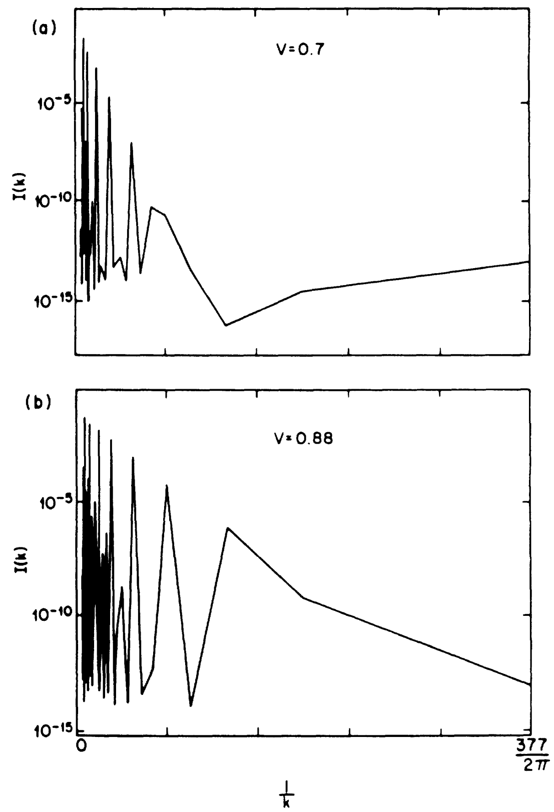

FIG. 10. Structure factor $I(k)$ plotted on a semilogarithmic scale vs $1/k$ for two values of $V<V_c$. The correlation length ξ is defined by fitting the envelope of the peaks to the form $I(k)=Ae^{-1/\xi k}$.

rithmic plot of $|\Gamma(k)|^2$ vs $1/k$ will exhibit a linear slope characteristic of the convergence rate of the perturbation theory; our data is plotted in this manner in Fig. 10, and the heights of the principal peaks appear to exhibit an envelope with linear dependence on $1/k$. The slope, which we define to be the inverse correlation length ξ^{-1} for the unpinned phase, is a measure of the length scale of the variations of $\Gamma(j)$. In Fig. 11 ξ^{-1} is plotted for various values of $|\epsilon|=|V-V_c|$, and it appears that $\xi\propto|\epsilon|^{-\nu'}$ with $\nu'=1.0\pm0.1$. The correlation length for $V<V_c$ is an order of magnitude smaller than for $V>V_c$, which we believe is due to arbitrary factors of $2\pi Q_n/P_n\cong 10$ in the definition of ξ for $V<V_c$.

By examining the difference between ground-state and lowest saddle solutions, we have found that one can define a correlation length that diverges on both sides of the transition like $|V-V_c|^{-\nu}$, with $\nu=\nu'=1.0$ equal to the finite-size scaling exponent $\bar{\nu}$, as expected.

One can find a physical interpretation of the correlation length in the unpinned phase. Recall that, as shown in Sec. II C, $1+dg/dx$ is the (unnormalized) eigenvector of the zero-frequency sliding mode in the unpinned phase. For small V, the sliding mode will involve motion which is spread out relatively uniformly over the whole chain, but as V increases, the motion will be concentrated more and more in smaller and smaller regions of the system until at V_c, an infinite amount of motion is needed at a countable number of points [corresponding to the step function structure of $x+g(x)$]. For $V\lesssim V_c$, the motion will be concentrated in separated regions. The characteristic maximum scale of the distances between these regions will be of order the correlation length ξ.

At least one more exponent is necessary to describe the pinning transition. This can be seen by examining Fig. 8, in which the difference between the ground-state and sad-

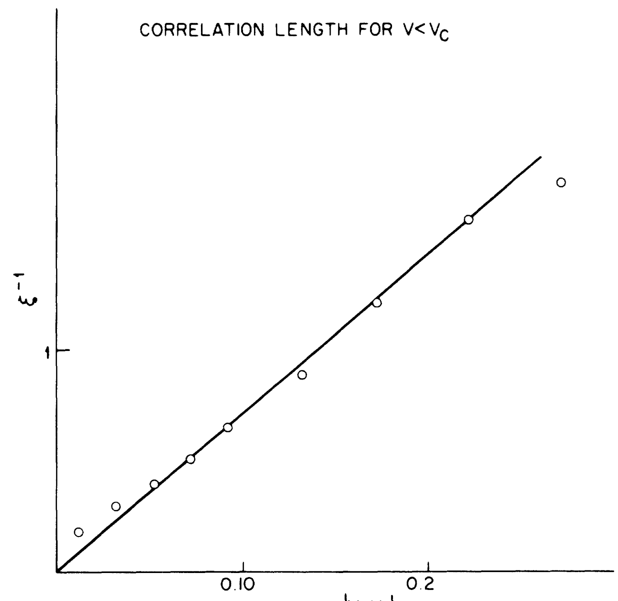

FIG. 11. Inverse correlation length plotted vs $|V-V_c|$, demonstrating that $\nu=1.0\pm0.1$ for $V<V_c$.

dle solutions $\Gamma(j)$ for 377 balls is plotted for $V < V_c$. The exponent $\sigma = 0.721$ describes the maximum of the curve, and $\nu = 1.0$ describes the length scale of variations in the curve. However, in order to describe the amplitude of the fluctuations in $\Gamma(j)$, one needs to know how the minimum of $\Gamma(j)$ varies with V. Shenker and Kadanoff[9] calculated this exponent in the unpinned phase by determining how close the ball nearest the bottom of a well is to the bottom, and they found that the distance from the bottom d_n for a P_n/Q_n cycle satisfies a scaling form

$$d_{3n+i} = (P_n)^{-\tau} D_i(\epsilon P_n^{1/\bar{\nu}}) \tag{4.9}$$

for $i = 0$, 1, and 2, with $\bar{\nu} = 1.0 \pm 0.015$ and $\tau = 1.093 \pm 0.001$. However, they found scaling only for every third approximant, i.e., three different scaling functions D_i, depending on whether P_n, Q_n, or both P_n and Q_n are odd. This complication probably reflects the fact that the balls near the top dominate at the transition, and the balls near the bottom may be merely reflecting the singularity of those at the top described by the exponent $\sigma = 0.721$. However, a detailed understanding of this scaling behavior is lacking and our numerical accuracy is not sufficient to determine whether the exponent τ also describes the behavior of the bottom balls in the pinned phase.

Several other quantities which we have not yet investigated in detail should show interesting scaling behavior near the pinning transition; examples include the phonon spectrum, the threshold field, and the density of metastable states. Aubry[6] has shown that this last quantity is zero in the unpinned phase, and it is nonzero in the pinned phase. A detailed study of these and other quantities should provide more insight into the physics of the pinning transition.

V. SPECULATIONS AND CONCLUSIONS

In this paper we have restricted our attention to a simple system with relative periodicity $\alpha = \phi = (1+\sqrt{5})/2$. On general grounds, one expects that other systems with the same periodicity but different potentials will be in the same universality class and exhibit the same critical behavior (in particular the same exponents). This will probably be true only if the potential is sufficiently smooth, i.e., if it has a sufficient number of continuous derivatives. It is not at all clear at this stage how smooth the potential must be, but a simple lower bound on the necessary smoothness is obtained by considering a periodic potential with a cusp (discontinuity in the first derivative), which has been shown to exhibit no unpinned phase[6(c)] and is thus in a different universality class from the analytic potential considered here. In order for the KAM theorem for the existence of an unpinned phase to be valid, more than three continuous derivatives are necessary, presumably setting a better lower bound on the necessary smoothness.

A more interesting question concerns the degree of universality for analytic potentials when the relative periodicity α is varied. Mackay[10] has shown that all irrationals whose continued fractions end in an infinite string of 1's have the same exponents. Shenker and Kadanoff[9] have calculated the exponents for $\sqrt{2}-1 = [0,2,2,2,\ldots]$ and found them to be within 1.5% of those for the golden mean, while our preliminary results using their methods (for $V < V_c$) for $\alpha = [1,2,1,2,\ldots]$ and $\alpha = [1,4,4,4,\ldots]$ indicate that the exponents for these periodicities are within 3% of those for the golden mean. However, the apparent numerical accuracy of $\sigma/\bar{\nu}$ is about 0.1%; it is not clear whether the variation is due to scaling corrections or to slight but significant differences between quadratic irrationals.

In any case, we conjecture that the exponents for all quadratic irrationals are similar. Preliminary calculations for $\alpha = [2,1,2,1,1,1,1,1,2,2,2,1,2,1,1,2]$, a random string of 1's and 2's, suggest (perhaps contrary to expectations) that power-law scaling behavior exists for this nonquadratic irrational with exponents within a few percent of those for $(\sqrt{5}+1)/2$.[19] If further study supports this conclusion, it may be that the "almost universality" as a function of α holds for all α approximable optimally to order $1/n^2$, a class which consists of all quadratic irrationals and all other irrationals with bounded entries in their continued fractions.

It would be interesting to investigate periodicities α with more rapidly converging rational approximants, although there may be technical difficulties in trying to use the finite-size scaling methods of this paper and other recent work. It seems reasonable to speculate that the exponents for all relative periodicities α which are not Liouville numbers are primarily determined by the convergence rate of the continued fraction of α.

A study of the exponents as a function of α is being carried out. Understanding their apparent weak dependence on relative periodicity and the apparent scaling behavior for nonquadratic irrationals is a challenging unsolved problem.[20]

Lastly we note that it is natural to assume that further-neighbor interactions between the balls do not change the critical behavior (at least not if they are reasonably weak). From this it follows that $2n$-dimensional area-preserving maps (see Appendix B) have the same critical behavior at the breakdown of an orbit with two incommensurate frequencies as the standard two-dimensional map with two frequencies.

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Note added. We have received a copy of unpublished work by Peyrard and Aubry[21] which also discusses scaling at the pinning transition, but examines only the pinned phase (they evaluate a correlation length, the minimum phonon frequency, the discommensuration pinning force, and the threshold electric field). Their definition of the correlation length is equivalent to ours for $V > V_c$, but they obtain $\nu = 0.960 \pm 0.004$ versus the value from Ref. 9, $\nu = 1.00 \pm 0.15$ (assuming $\nu = \nu' = \bar{\nu}$). Their value was obtained by examining a 377-ball system only, and we believe that the discrepancy may be due to corrections to scaling. The finite-size effects are negligible only if the correlation length is less than 100 or so ($V \gtrsim 1.0V_c$); but on the other hand, outside the scaling region when ϵ is small, there are corrections to scaling. Examination of the scaling function for the disorder parameter ψ shows deviations when $V \sim (1.13)V_c$ even in the infinite system. Since Peyrard and Aubry include data in the range V_c to $\sim 5V_c$ and obtain ν from a fit between V_c and $2V_c$, they may be incorrectly weighting data outside the scaling region, which would account for the discrepancy. Mackay[10] has recently calculated the exponents σ and ν very accurately, both directly and also by finding eigenvalues about a renormalization-group[22] critical fixed-point map. He finds $\sigma = 0.712$ and $\nu = 0.987$.

Mather[23] has recently considered comparing the energies of the ground-state and lowest saddle solutions (which he calls the max and minimax solutions) for a sequence of Q_n/P_n's. He proves rigorously that this procedure has a well-defined incommensurate limit, and that pinning is equivalent to the statement that the ground state and saddle state have different energies in this limit. This conclusion is compatible with our results and those of Aubry. Previous work on the unpinned phase of this model by Sacco and Sokoloff[24] has also been brought to our attention by Sokoloff.

APPENDIX A

A principal property of irrational numbers with which we are concerned is how well they can be approximated by rationals.[25] For instance, in the context of the small denominators found in the weak potential perturbation theory for a given α, one wishes to know how close $|n\alpha - m|$ is to zero for a given integral n (corresponding to the order of the perturbation theory) and optimally chosen integral m. We quote here several useful results.[25]

Definition: If $f(n)$ is a positive, monotonically decreasing function, α is *approximable to order* $f(n)$ if there is a constant C_1, such that the condition

$$|\alpha - m/n| < C_1 f(n) \tag{A1}$$

is satisfied for an infinite number of integral m and n. An irrational α is *optimally approximable* to order $f(n)$ if in addition there is another constant $C_2 < C_1$ such that

$$|\alpha - m/n| < C_2 f(n) \tag{A2}$$

has only a finite number of solutions (i.e., for every function $g(n)$ with α approximable to order $g(n)$, $\lim_{n\to\infty}[g(n)/f(n)] > 0$).

(1) All irrationals can be approximated to order $1/n^2$.

(2) *Quadratic irrationals* [those of the form $\alpha = (a + b\sqrt{r})/d$, with a,b,r,d integers] are optimally approximable to order $1/n^2$.

(3) If the sum

$$S_f = \sum_{n=1}^{\infty} n f(n) \tag{A3}$$

is infinite, then almost all (in the sense of Lebesgue measure) irrationals are approximable to order $f(n)$.

(4) Conversely, if S_f is finite, than almost no irrationals (a set of measure zero) are approximable to order $f(n)$.

For example, the sets of irrationals *optimally* approximable to order $1/n^2$ or $1/(n^2 \ln n)$ have zero measure while those approximable to order $1/[n^2(\ln n)^2]$ or $1/n^{2+\epsilon}$ (with $\epsilon > 0$) have zero measure.

In particular, the *Liouville numbers*, which are approximable to order $1/n^{\mu}$ for any μ, are a set of zero measure (although they are dense). The KAM theorem applies to all α that are not Liouville numbers.

The best rational approximations to α with given bounds on the denominators are obtained from truncations of the continued fraction expansion of α, which has the form

$$a_0 + \cfrac{1}{a_1 + \cfrac{1}{a_2 + \cfrac{1}{a_3 + \cdots}}}\ , \tag{A4}$$

where the a_j are positive integers (except a_0, which is zero for $0 < \alpha < 1$).

The sequence $\{a_j\}$ is infinite if and only if α is irrational. For irrational α the continued fraction expansion is unique. In order to obtain the sequence of best approximants $\{Q_n/P_n\}$ to α,[18] the continued fraction is truncated by setting $a_{n+1} = \infty$; i.e.,

$$\frac{Q_n}{P_n} = a_0 + \cfrac{1}{a_1 + \cfrac{1}{a_2 + \ddots + \cfrac{1}{a_n}}}\ . \tag{A5}$$

Given a continued fraction which we denote $[a_0, a_1, \ldots, a_j, \ldots]$, the integers P_i and Q_i of the approximants are determined recursively by

$$\begin{aligned} &P_{-1} = 0\ ,\quad P_0 = 1\ ,\quad P_i = a_i P_{i-1} + P_{i-2}\ ,\\ &Q_{-1} = 1\ ,\quad Q_0 = a_0\ ,\quad Q_i = a_i Q_{i-1} + Q_{i-2}\ . \end{aligned} \tag{A6}$$

The "odd" approximants Q_{2j+1}/P_{2j+1} are always greater than α, but decrease as j increases, while the even approximants are always less than α, but increase with j. It can be shown that

$$\frac{Q_j}{P_j} - \frac{Q_{j-1}}{P_{j-1}} = \frac{(-1)^{j-1}}{P_j P_{j-1}}\ , \tag{A7}$$

so that as $j \to \infty$ the sequence of approximants converges to α.

The order to which α is approximable, i.e., how fast its best approximants converge, is related to the behavior of the high-order coefficients of its continued fraction expansion. The set of numbers with bounded continued fractions corresponds exactly to those numbers which can be optimally approximated to order $1/n^2$.

All quadratic irrationals have periodic continued fractions and hence their rational approximants converge slowly and smoothly; it is for this reason that we study a quadratic irrational in this paper. The number whose rational approximants converge most slowly is the golden mean $\phi = (\sqrt{5}+1)/2$, whose continued fraction is $[1,1,1,\ldots]$.

APPENDIX B: RELATIONSHIP TO THE STANDARD MAP OF DYNAMICAL SYSTEMS THEORY

Dynamical systems with competing periodicities, such as an anharmonic oscillator with a "natural" frequency ω_1 externally forced at a frequency ω_2, have been extensively studied recently.[7–11] A model for this system is the so-called "standard map"

$$r_{j+1}=r_j+V\sin\theta_j\ , \tag{B1a}$$

$$\theta_{j+1}=\theta_j+r_{j+1}\ , \tag{B1b}$$

with the index j representing discretized time, which we have seen is equivalent to Eq. (2.1). The relative periodicity is called the winding number in this context.

Several authors[1,12] have tried to exploit the relation between these systems in order to explore the pinned phase of the discrete Frenkel-Kontorova model. However, because of questions of stability, naively carrying over results from the standard map leads to very misleading results. In this appendix we discuss the relation between properties of various solutions of Eqs. (2.1) and (B1) in order to elucidate the correspondence, in particular as implied by Aubry's work.[6]

An important question concerning any solution to Eqs. (B1) is whether the solution is stable to small perturbations. For the balls connected by springs, a sufficient (and necessary) condition for local stability is that the Hessian of the Hamiltonian, $\partial^2 H/\partial X_i \partial X_j$, have only non-negative eigenvalues. Physically, this means that no small displacements of the balls from their positions can lower their energy. However, when (B1) is viewed as a time evolution, the stability condition is different, as shown below.

One can start an oscillator with the initial velocity and position given, thus determining θ_1 and r_1. Equations (B1) then determine θ_j and r_j for all j, i.e., the initial conditions determine the position of the oscillator at all future times. A solution is called "elliptic" if the changes $\delta\theta_j,\delta r_j$ induced in θ_j and r_j by a small perturbation $\delta\theta_1,\delta r_1$ to θ_1 and r_1 are uniformly small for all j. The elliptic solutions are particularly important physically because two experiments with nearly identical initial conditions will yield nearly identical results for all times. However, there also exist solutions for which almost all small perturbations grow without bound at long times; these are called "hyperbolic." The condition for ellipticity of an orbit can be written in terms of the linearized transformation T_j about a solution with initial conditions θ_1,r_1 defined by

$$\begin{bmatrix}\delta\theta_j\\ \delta r_j\end{bmatrix}=T_j\begin{bmatrix}\delta\theta_1\\ \delta r_1\end{bmatrix}. \tag{B2}$$

Since the map is area preserving, T_j generally has determinant 1. The solution is elliptic if the eigenvalues of T_j both have modulus 1 in the limit of large j.

Thus the criterion for the stability of the balls and springs and the criterion for the ellipticity of the orbit in the phase space of the oscillator are quite different. In fact, unless a zero-frequency phonon mode exists, physically stable states of the balls are always equivalent to hyperbolic orbits. This result, which we discuss below, is implied by Greene's work.[8]

Again, we consider approximating an orbit with irrational winding number by a sequence of orbits with period $\{P_n\}$. It is straightforward to show that the linearized transformation about this orbit is, with $j=P_n$,

$$T_{P_n}=\begin{bmatrix}1+V\cos\theta_{P_n-1} & 1\\ V\cos\theta_{P_n-1} & 1\end{bmatrix}\begin{bmatrix}1+V\cos\theta_{P_n-2} & 1\\ V\cos\theta_{P_n-2} & 1\end{bmatrix}\cdots\begin{bmatrix}1+V\cos\theta_1 & 1\\ V\cos\theta_1 & 1\end{bmatrix}. \tag{B3}$$

If the eigenvalues of T_{P_n} both are of modulus 1 for $n\to\infty$, then the orbit is elliptic. This condition can be conveniently written in terms of the trace of T_{P_n}. Greene defines the *residue*

$$R_n=\tfrac{1}{4}(2-\mathrm{Tr}T_{P_n})\ , \tag{B4}$$

whence the condition for ellipticity is that

$$0\le R_n\le 1 \tag{B5}$$

for large n. The residue is simply related to the product of the phonon frequencies for the system of P_n balls with periodic boundary conditions,

$$R_n=-\tfrac{1}{4}\prod_{j=1}^{P_n}\omega_j^2\ , \tag{B6}$$

i.e., to the determinant of the force matrix $\overleftrightarrow{\mathrm{M}}$ (with periodic boundary conditions) defined in Sec. II A, which is just the Hessian of the Hamiltonian.[8] The residue R of an orbit with irrational winding number is just the limit of R_n as $n\to\infty$. It follows that any stable or metastable state will have $R\le 0$. If $R=0$, then an elliptic state with a zero-frequency phonon can exist, but stable or metastable systems of balls with no zero-frequency phonon have $R<0$ and hence correspond to hyperbolic orbits.

Physically, this result says that given a pinned stable or metastable state, no nearby solution to the force equations exists with the same periodicity. Most perturbations to θ_1 and r_1 cause the periodicity to change, which results in arbitrarily large displacements far from θ_1.

For sufficiently small potential only two solutions exist for a given rational winding number, Q_n/P_n. The ground-state solution is hyperbolic and the saddle-state solution is elliptic. As n increases and Q_n/P_n approaches the irrational α, the two solutions meld into one KAM surface. This orbit with winding number α has zero residue and is hence elliptic.

At $V_c(\alpha)$ the elliptic KAM orbit disappears, and for $V>V_c(\alpha)$, it is observed numerically that all orbits with winding number α are hyperbolic. Physically this result is supported by the behavior of the saddle state. For $V>V_c$, the saddle solution has a ball at the top of a well that is "held up" by symmetry only, so an infinitesimal change in the ball next to the one at the top causes the position of the one at the top to change by a finite amount as it "falls down." The saddle solution which corresponded to an elliptic state for $V<V_c$ has thus become hyperbolic for $V>V_c$. The residue of the rational approximating orbits will approach $+\infty$ as $n\to\infty$ for $V>V_c$.

For $V>V_c$ the inverse correlation length ξ^{-1} is the Lyapunov exponent of the dynamical system. From the definition of the correlation length in the pinned regime (Sec. III), it is apparent that one of the eigenvalues, Λ_j^-, of the linearized transformation T_j about the ground-state solution goes as $e^{-j/\xi}$ for large j. Since T_j has determinant one, its other eigenvalue Λ_j^+ goes as $e^{+j/\xi}$. The Lyapunov exponent λ is given by

$$\lambda \equiv \lim_{j\to\infty} \frac{1}{j}\ln\Lambda_j^+ = \xi^{-1} \, . \tag{B7}$$

For $V>V_c(\alpha=\phi)$, the standard map is in the chaotic regime. Only very special initial conditions, which apparently have no physical meaning for dynamical systems, will lead to quasiperiodic orbits like the ground state of the balls.

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[1]See, for example, P. Bak, Rep. Prog. Phys. 45, 587 (1982) and references therein.

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[6]S. Aubry (with various collaborators) has written a large number of important papers on this topic with some overlap in content. His early work on studies of the ground state is unfortunately unpublished. We list here Aubry's published papers relevant to this subject. (a) S. Aubry, in *Solitons and Condensed Matter,* edited by A. Bishop and T. Schneider, Vol. 8 of *Solid State Sciences* (Springer, Berlin, 1978), pp. 264—278; (b) in *Some Non-Linear Physics in Crystallographic Structure,* Vol. 93 of *Lecture Notes in Physics* (Springer, Berlin, 1979), pp. 201—212; (c) S. Aubry and G. André, Ann. Israel Phys. Soc. 3, 133 (1980); (d) S. Aubry, in *Intrinsic Stochasticity in Plasmas,* edited by G. Laval and D. Gresillon (Edition de Physique, Orsay, 1979), pp. 63—82; (e) Ferroelectrics 24, 53 (1980); (f) in *The Devil's Staircase Transformation in Incommensurate Lattices,* Vol. 925 of *Lecture Notes in Mathematics* (Springer, Berlin, 1982), pp. 221—245; (g) in *Symmetries and Broken Symmetries,* edited by N. Boccara (Idset, Paris, 1981), pp. 313—322; (h) in *Numerical Methods in the Study of Critical Phenomena,* edited by J. Della Dora, J. Demongeot, and B. Lacolle (Springer, Berlin, 1981), pp. 78, 79; (i) in *Physics of Defects, Les Houches, Session XXXV,* 1980, edited by R. Balian, M. Kleman, and J. P. Poirier (North-Holland, Amsterdam, 1981), pp. 431—451; (j) F. Axel and S. Aubry, J. Phys. C 14, 5433 (1981).

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[10]R. S. Mackay, Ph.D. thesis, Princeton University, 1982 (unpublished).

[11]The literature on the standard map is extremely extensive; see, for example, J. M. Greene, R. S. Mackay, F. Vivaldi, and M. J. Feigenbaum, Physica D 3, 468 (1981) and references therein.

[12]P. Bak, Phys. Rev. Lett. 46, 791 (1981); see also Ref. 1.

[13]A. N. Kolmogorov, Dokl. Akad. Nauk SSSR 98, 527 (1954); V. I. Arnold, Usp. Mat. Nauk 18, 91 (1963); J. Moser, in *Stable and Random Motions in Dynamical Systems,* Annals of Mathematics Studies #77 (Princeton University Press, Princeton, 1973).

[14]Aubry and André (see Ref. 6) have considered this point and proven some results on the nature of the $\omega=0$ eigenvector, but they have not demonstrated analytically that the balls slide (though they find the result numerically).

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[18]We study systems with relative periodicity $\alpha>1$ and call its approximants Q_n/P_n with $Q_n>P_n$. Other recent authors (e.g., Ref. 20) have considered $\alpha<1$ with approximants P_n/Q_n with again $Q_n>P_n$. For the golden mean $\alpha=\phi$ the approximants for $\phi-1$ considered in Ref. 20 (which is exactly equivalent to ϕ) are just the reciprocals of those for ϕ considered here. The notation difference will thus hopefully not cause confusion.

[19]It may be that, rather than the simple power-law behavior for quadratic irrationals, the exponents generally need to be defined in a more complicated way: for example, for each α,

$$\limsup_{V\to V_c} \xi(V)\,|V-V_c|^{\nu_\alpha}=A_1 \, ,$$

$$\liminf_{V\to V_c} \xi(V)\,|V-V_c|^{\nu_\alpha}=A_2 \, ,$$

with $\infty>A_1\geq A_2>0$ nonuniversal but ν only depending on α. This allows for the possibility of a badly defined amplitude of the singularity. However, preliminary evidence for $\alpha=[2,1,2,1,1,1,1,1,2,2,2,1,2,1,1]$ suggests that this problem may not arise.

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