Devil's staircase in a one-dimensional model

Amitava Banerjea* and P. L. Taylor
Department of Physics, Case Western Reserve University, Cleveland, Ohio 44106
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A one-dimensional model of a chain of canted arrows in an external field is proposed to describe some quasi-one-dimensional systems, e.g., spin-, charge-, and mass-density-wave systems, and helical polymers. The chain has a natural cantedness measured by an angle α, and is also subject to an externally applied aligning field of strength γ. At $T=0$, the α-γ phase diagram has an infinite number of commensurate phases, and the variation with α of the mean angle between nearest-neighbor arrows has the form of a devil's staircase for all γ. The transfer-integral technique is used to calculate the Helmholtz free energy and the order parameter of the system as functions of temperature. No sharp transitions occur at $T>0$, but some of the features of the $T=0$ phase diagram persist at low temperatures. Transitions occur from one phase to another when the energy required to create a kink in one phase becomes zero. The equations determining the minimum-energy configurations are rewritten so as to define a two-dimensional area-preserving mapping; fixed points and invariant curves are found for this mapping. Invariant curves are either smooth and continuous or chaotic. The relation of the nature of the invariant curves to the question of the completeness of the devil's staircase is discussed.

I. INTRODUCTION

A great deal of attention has been focused in recent years on certain materials which show incommensurate-commensurate (I-C) phase transitions and elaborate phase diagrams. Such I-C phase transitions have been observed in some spin-density-wave (SDW) systems, e.g., cerium antimonide,[1-3] and charge-density-wave (CDW) systems, e.g., tetrathiofulvalene tetracyano-p-quinodimethane (TTF-TCNQ) and $K_2Pt(CN)_4Br_{0.30}\cdot 3H_2O$ (KCP).[4-8] Another interesting material that exhibits such I-C transitions is the crystalline polymer polytetrafluoroethylene (PTFE),[9-12] which consists of linear sequences of CF_2 units. At atmospheric pressure the stable configuration of the chains has the CF_2 units arranged on a helix. As the temperature and pressure are varied, the material undergoes phase transitions between phases in which the pitch of the helix is commensurate with the axial distance between successive CF_2 units and phases in which the two lengths are incommensurate.[9-12]

A variety of phenomenological models have been proposed to describe such systems.[12-30] These models show some of the interesting behavior of the real experimental systems as well as some other fascinating features. One of the most widely studied of these model systems is a model first proposed by Kontorova and Frenkel[13] to describe defects in solids. This model, known variously as the Frenkel-Kontorova model, the Frank and van der Merwe model,[14] and the discrete sine-Gordon model, has been studied by a number of authors and applied to a wide variety of physical problems. This and most other models belong to a general class of models which has recently been studied by Aubry.[25-30] In this paper we present a new model which can be applied to a variety of systems such as helical ferromagnets, certain ferroelectrics, and to some helical polymers, e.g., PTFE. This model in its most general form does not satisfy all the conditions required of the class of systems studied by Aubry. In particular, the near-neighbor potential in this model is not convex everywhere, as is required of Aubry's class of models. In this paper, however, we confine our attention to the convex region of the potential and investigate the behavior of the model subject to this constraint. The deviation from convexity introduces the possibility of interesting new consequences and we hope to investigate these later.

We present the results of our studies in three main parts. Section II contains a description of the model and the properties of the ground state of the system at zero temperature. A discussion of the behavior of the system at finite temperatures and of the role of kinks in determining phase transitions is presented in Sec. III. Finally, in Sec. IV we reformulate the equations for a minimum-energy solution in the form of a two-dimensional mapping and study the invariant curves of this mapping. We demonstrate the existence of smooth invariant curves which undergo transitions to chaotic sets of points and discuss the relevance of this behavior to the completeness of the devil's staircase.

II. MODEL

The model that we have studied may be visualized as a linear array of canted "arrows" or "spins" of equal size, each free to rotate in a plane perpendicular to the line joining the arrows as shown in Fig. 1. The angle that the jth arrow makes with a certain fixed direction, defined as the z direction, is ϕ_j. Each arrow interacts with its nearest neighbors with a potential energy of the form

$$W(\phi_{n+1},\phi_n) = -\cos(\phi_{n+1}-\phi_n-\alpha) \ . \tag{1}$$

Here, α is a measure of the degree of natural cantedness of the system. In order to minimize this nearest-neighbor energy, in the absence of other forces, the arrows form a helix, and α is a measure of the pitch of that helix. This potential, unlike other similar potentials which have been studied in the past,[13–30] is smoothly periodic in the variables of interest, i.e., in ϕ_n and ϕ_{n+1}.

The arrows are also subject to an external symmetry-breaking field, and the potential energy of the jth arrow in the presence of this field is given by

$$V(\phi_j) = -\gamma\cos(2\phi_j) \ . \tag{2}$$

Here, γ is a measure of the strength of the external field relative to that of the nearest-neighbor interaction. Under the influence of this external field alone, i.e., with no nearest-neighbor interaction, the ground-state configuration would have all the arrows aligned parallel or antiparallel to the z direction.

Ignoring kinetic-energy terms, we may express the total Hamiltonian for the array of arrows as

$$\begin{aligned} H &= \sum_n W(\phi_{n+1}-\phi_n) + V(\phi_n) \\ &= -\sum_n [\cos(\phi_{n+1}-\phi_n-\alpha)+\gamma\cos(2\phi_n)] \ . \end{aligned} \tag{3}$$

This potential is not convex everywhere; its mixed second derivative is not negative definite, as is required of the class of systems studied by Aubry.[25–30] However, while the nonconvexity of the potential may well introduce new possibilities, it is not unreasonable to assume that the low-energy configurations of the system do not stray far outside the regions of convexity of the potential in Eq. (1). It is clear that for $\gamma=0$, any deviation into the nonconvex regions of the nearest-neighbor potential results in an increase in energy and cannot be preferred. This is also expected to hold for small values of γ, and it appears unlikely that for any value of γ the configurations that lie mostly in the nonconvex regions of the potential will be ground-state configurations.

It is to be expected that different versions of the system where the value of the parameter α differs by an integral multiple of π will show similar behavior. In order to include all such systems in this one discussion it is convenient to define, corresponding to the variable α, a modified variable,

$$\tilde{\alpha} = \alpha - m\pi \ , \tag{4}$$

so that $\tilde{\alpha}\in[-\pi/2,\pi/2]$.

III. ZERO-TEMPERATURE BEHAVIOR

We may now proceed to determine what the configuration of arrows is in the ground state for given values of α and γ. The ground-state configuration can be either commensurate or incommensurate. A configuration, or phase, is said to be commensurate if for all integers i it is true that

$$\phi_{i+p} = \phi_i + m\pi \ , \tag{5}$$

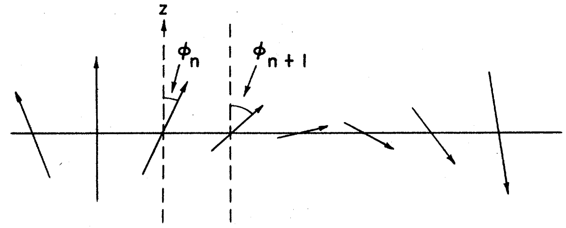

FIG. 1. Schematic drawing of the model system of arrows on a string.

where m is an integer independent of i. The smallest positive integer p that satisfies Eq. (5) is called the order of commensurability of the phase. Otherwise the configuration is said to be incommensurate. At this time it is convenient to define an average angular separation between nearest-neighbor arrows, c, as follows,

$$c = \lim_{N\to\infty}\left[\frac{1}{2N\pi}\sum_{n=-N}^{N}(\phi_{n+1}-\phi_n)\right] \ . \tag{6}$$

For a commensurate configuration, c is a rational number, while for an incommensurate configuration it is an irrational number.

It is obvious that for $\gamma=0$, the ground-state configuration is one in which $c=\alpha/\pi$, and the configuration is or is not commensurate depending on whether α is or is not a rational fraction of π. It is also obvious that for any value of α, we will find that $c=0$ when $\gamma\gg1$. This configuration is conveniently visualized as one in which alternate arrows are parallel and antiparallel to the z direction. For nonzero α, as γ is lowered, there must then be a transition from this configuration to one in which $c=\alpha/\pi$. This transition may occur directly as a first-order transition or a continuous one, or it may occur in a series of steps with the system passing through several other stable intermediate configurations.

The conditions for a ground-state configuration are given by the infinite set of coupled equations:

$$\sin(\phi_{n+1}-\phi_n-\alpha)-\sin(\phi_n-\phi_{n-1}-\alpha) = 2\gamma\sin(2\phi_n) \ . \tag{7}$$

Solutions to Eq. (7) yield configurations for which the energy is a local extremum. Of these, a subset are minimum-energy configurations and a further subset of these are the ground-state configurations. Our objective is to determine the nature and properties of the true ground-state configurations.

That the infinite set of equations represented by Eq. (7) forms a set of recursion relations for the ϕ's can be seen more clearly by rewriting them as

$$\phi_{n+1} = \phi_n + \alpha + \arcsin[\sin(\phi_{n+1}-\phi_n-\alpha)+2\gamma\sin(2\phi_n)] \ . \tag{8}$$

The ambiguity in the interpretation of the inverse sine is removed by our decision to remain within the convex region of the nearest-neighbor potential, which requires that we restrict ourselves to the principal branch of the inverse sine.

Two angles, e.g., ϕ_0 and ϕ_1, still remain undetermined by these equations. These degrees of freedom cannot be eliminated without the imposition of further constraints on the system. One meaningful way to eliminate one of the degrees of freedom is to impose on the system a value of c and so obtain a solution set $\{\phi_i\}$ with energy E which depends on the value of c. One can then minimize E with resepct to c and thus obtain the ground-state configuration $\{\phi_i^G\}$. We have used this approach though it has not been possible to obtain an analytical solution set $\{\phi_i\}$ or an analytical expression for $E(c)$. We have considered different commensurate configurations of increasing order, thereby imposing rational values of c, and have minimized the energy in each. Then for given α and γ, we have assigned the commensurate phase with the lowest energy to be the ground state.

One major handicap of this method is that one cannot strictly rule out the possibility of there being incommensurate phases with lower energy than the commensurate phases that we can consider. However, from the experience of rigorous studies on other similar potentials,[19,25,26] it appears very unlikely that such incommensurate phases will occupy a large part of the phase diagram of this system. We will return to this problem later when we discuss the question of the completeness of the devil's staircase.

One can write a general solution to Eq. (8) in the form

$$\phi_n = \left[nc + d + \sum_k t_k \sin\pi(nq_k + e_k) \right] \pi , \tag{9}$$

where $c\pi$ is the average separation between arrows as defined in Eq. (4), where $d\pi$ is an overall displacement with respect to the z direction, and where the remaining term is a modulation. For a commensurate configuration with order of commensurability p, it is easy to see that c and q_k must be of the form $2p_1/p$. Then, for the four lowest-order commensurate phases, only one term in the series survives, and the solution is of the form

$$\phi_n = \{ nc + d + t \sin[\pi(nc + e)] \} \pi . \tag{10}$$

The minimum-energy solution can now be found by minimizing the energy with respect to c, d, t, and e. This analytical approach is tractable[31] only for commensurate phases of orders 1 and 2, and, to some extent, for the commensurate phase of order 3. For higher-order commensurate phases the mathematics becomes too involved and one must resort to numerical techniques and directly minimize the energy with respect to the p independent variables $\{\phi_1, \phi_2, \ldots, \phi_p\}$. We have checked that, for the commensurate phases of orders 1, 2, and 3, the two methods outlined here yield the same results.

Figure 2 shows plots of energy against α' $(=\alpha/\pi)$ for different low-order commensurate phases at different values of the strength of the external field, γ. Results have been shown for the range $0<\alpha'<0.5$ because the curves are symmetrical about $\alpha'=0$ and 0.5. The resulting phase diagram is shown schematically in Fig. 3. It is clear that phases with higher orders of commensurability interpose themselves in the regions between neighboring phases with lower orders of commensurability. Also, as γ is increased, the regions over which the higher-order commensurate phases are stable become narrower. This might suggest that each high-order commensurate phase ceases

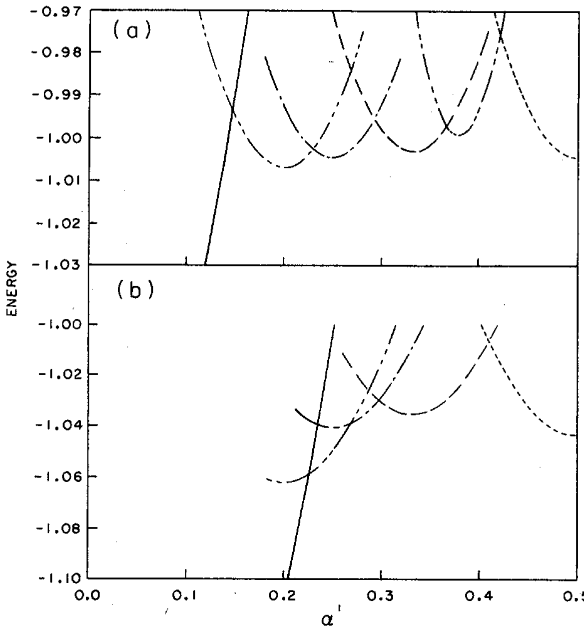

FIG. 2. Energy per arrow plotted against α' for commensurate phases of orders 1 (solid line), 2 (dotted line), 3 (dashed line), 4 (dotted-dashed line), and 5 (double-dotted—dashed line) at (a) $\gamma=0.10$ and (b) $\gamma=0.30$.

to be stable above some value of γ and that a large number of triple points exist in the phase diagram. This is what had been reported by Ying[30] in his investigation of the discrete sine-Gordon system. However, we have

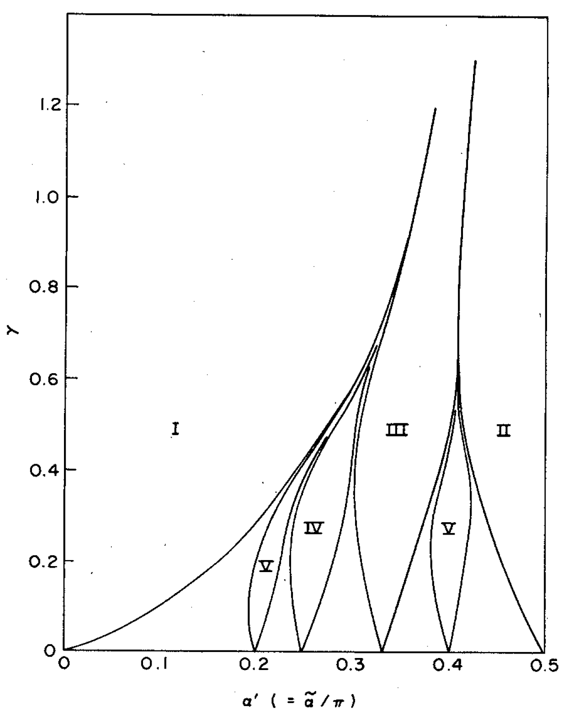

FIG. 3. Schematic α-γ phase diagram for the model system. Roman numerals indicate order of commensurability of the ground-state configuration.

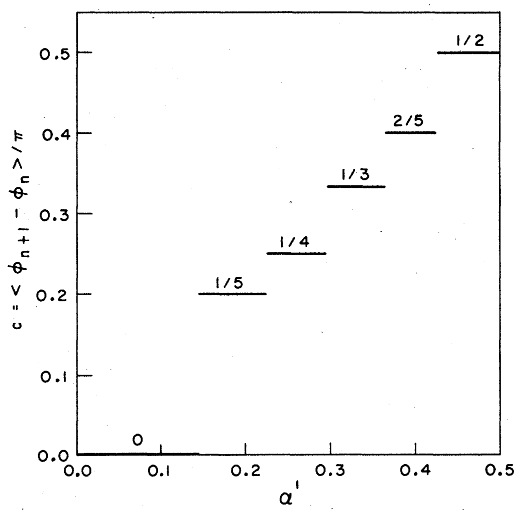

FIG. 4. Plot of c $(=\langle \phi_{n+1}-\phi_n \rangle/\pi)$ against α' at $\gamma=0.10$. Only commensurate phases with orders less than or equal to 5 have been considered.

looked into this question very closely and have been unable to find any triple points. All commensurate phases exist at all values of γ. As γ is increased, the phase diagram is dominated by the first-order commensurate phase, and all the higher-order phases are squeezed into a narrow region around $\alpha'=\frac{1}{2}$. A representative plot of c against α' is shown in Fig. 4. It is evident that the curve is indeed a devil's staircase.

IV. FINITE TEMPERATURES

As expected, there are no sharp phase transitions at $T>0$ in this one-dimensional system. However, at sufficiently low temperatures some features of the zero-temperature phase diagram do persist and the behavior of the system at low temperatures provides useful information about the nature of the transitions that occur at zero temperature. In particular, the lower-order commensurate phases tend most strongly to retain some order, and quasiordered forms of these phases can be identified at low temperatures. We have used the transfer-integral technique[32,33] in order to calculate the Helmholtz free energy of the system and the distribution of the angles ϕ, as functions of the temperature.

It can be shown[32,33] that for a one-dimensional array of arrows with nearest-neighbor interactions and a Hamiltonian of the form

$$H=\sum_n U(\phi_{n+1},\phi_n) , \tag{11}$$

the free energy per arrow can be obtained in the thermodynamic limit from a solution of the eigenvalue integral equation,

$$\lambda\psi(\phi)=\int \exp[-\beta U(\phi,\phi')]\psi(\phi')d\phi' . \tag{12}$$

The free energy F is given by

$$F=-\frac{1}{\beta}\ln\lambda_M , \tag{13}$$

where $\beta=(k_B T)^{-1}$, where k_B is Boltzmann's constant and λ_M is the eigenvalue of largest modulus ($|\lambda_M|>|\lambda_i|$ for all $i\neq M$). The distribution function $n(\phi)$ for the angle ϕ is given by

$$n(\phi)=\frac{\psi(\phi)\tilde{\psi}(\phi)}{\int \psi(\phi')\tilde{\psi}(\phi')d\phi'} , \tag{14}$$

where ψ_M and $\tilde{\psi}_M$ are the right and left eigenvectors associated with λ_M, respectively.

Once again, an analytical solution of the integral equation has proved elusive and we have had to resort to numerical solutions. In order to do this the integral eigenvalue equation must be converted to a matrix eigenvalue equation with the variable ϕ being permitted to assume a number, m, of equally spaced values in the range $[-\pi,\pi)$. This form of the model is usually referred to as the m-state version of the model. We have used a 36-state version of the model where ϕ has been allowed to change in steps of 10° in the range [−180°, 170°].

Figure 5 shows graphs of the free energy against α' for two values of γ at $\beta=100$. The absence of any sharp features and the lack of evidence for any sharp transitions are obvious. The structure that is present in this graph becomes clearer from Fig. 6 which shows the derivative of the free energy with respect to α' plotted against α' for the same values of γ as in Fig. 5, again at $\beta=100$. The solid triangles are the points obtained from numerical differentiation of the data of Fig. 5. Evidence of some transitions can be seen. However, as expected, these transitions are not sharp. At low temperatures it is reasonable to assume that the derivative of the free energy, $\partial F/\partial\alpha'$, is essentially identical to the derivative of the energy, $\partial E/\partial\alpha'$. The solid lines in Fig. 6 are plots of the analyti-

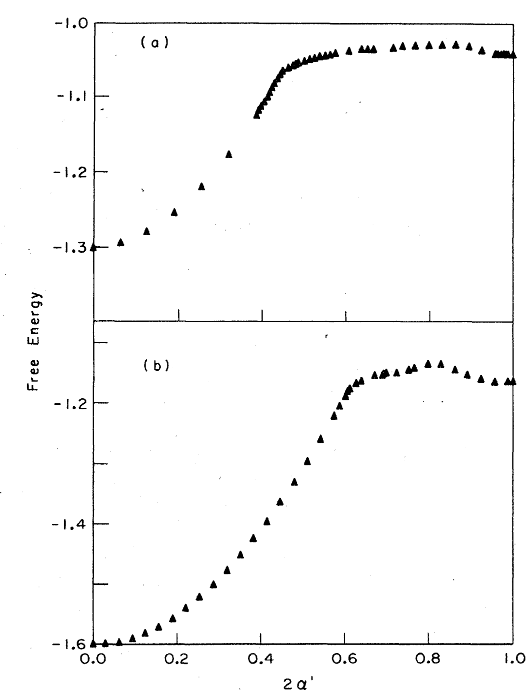

FIG. 5. Free energy as a function of α' at $\beta=100$ and (a) $\gamma=0.30$ and (b) $\gamma=0.60$.

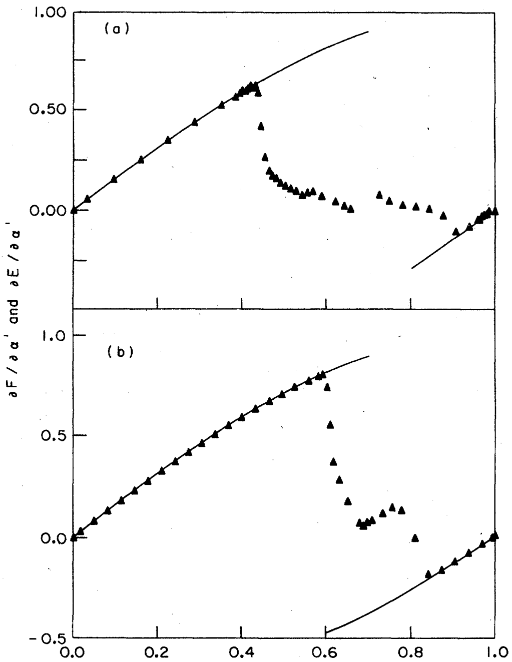

FIG. 6. $\partial F/\partial\alpha'$ (solid triangles) at $\beta=100$ and plots of $\partial E/\partial\alpha'$ (solid lines) for commensurate phases of orders 1 (I) and 2 (II) as function of α' at (a) $\gamma=0.30$ and (b) $\gamma=0.60$.

cal expressions for $\partial E/\partial\alpha'$ in the commensurate phases of orders 1 and 2. The agreement between the points and the solid lines over certain ranges of α' is striking. It is evident that over these ranges at this low temperature the disorder in the system is very small and the system is essentially in the commensurate phase that is the ground state at zero temperature.

In the first-order commensurate phase, ϕ_n is either 0 or π. A simple kink in such a system represents a smooth transition between the neighboring ground-state values of 0 and π. It is obvious that such a kink must pass over the potential barrier at $\phi=\pi/2$. It is then reasonable to assume that at sufficiently low temperature the number of arrows with $\phi=\pi/2$ is proportional to the number of kinks.[34,35] We may also assume that the density of kinks is sufficiently low that we may neglect any interaction be-

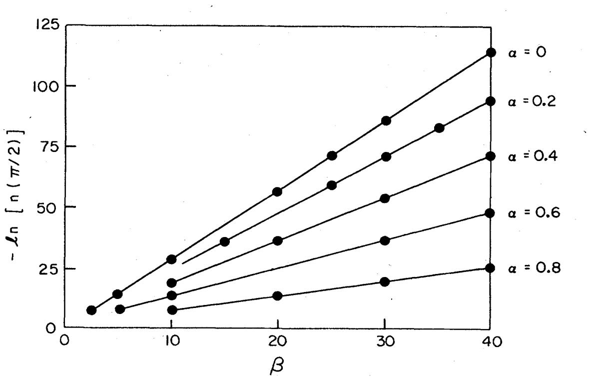

FIG. 7. Graphs of $-\ln[n(\pi/2)]$ against β for different values of α at $\gamma=0.60$.

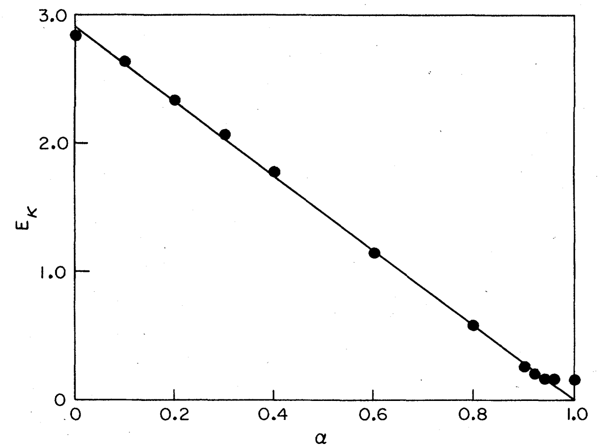

FIG. 8. Plot of E_k (as obtained from Fig. 9) against α in the first-order commensurate phase at $\gamma=0.60$.

tween them and assume that the number of kinks is governed by the Boltzmann distribution law,

$$n_{\text{kink}} \propto \exp(-\beta E_k)\ , \tag{15}$$

where E_k is the energy required to create an isolated kink. Consequently, one expects that for large values of β, i.e., for low temperatures, a plot of $-\ln[n(\pi/2)]$ against β will be a straight line with slope equal to E_k. At higher temperatures the system becomes increasingly disordered and a discussion in terms of kinks is no longer meaningful.

Figure 7 shows plots of $-\ln[n(\pi/2)]$ against β for different values of α at $\gamma=0.60$ in the range where the first-order commensurate phase is the most stable. Figure 8 shows the slopes of the straight lines in Fig. 7, i.e., E_k, plotted against α. One can see that the energy required to create a kink in the first-order commensurate phase decreases as α is increased from zero and vanishes at the value of α that marks the transition from the first-order commensurate phase to some other phase. Close to this point the interactions between kinks becomes increasingly significant and the curve begins to deviate from its linear behavior. A similar analysis for the second-order phase yields essentially similar results. It is clear from this analysis that the transition from one commensurate phase to another commensurate phase (or to an incommensurate one) occurs when the energy necessary for creating a kink in the first phase vanishes.

V. MAPPING

The equation determining the condition for a ground state, Eq. (8), can be transformed into two sets of coupled nonlinear difference equations involving only first differences by a procedure analogous to that used in deriving the Taylor-Chirikov[36] map from the equations governing the discrete sine-Gordon system. In order to do this we define a new variable s_n through the equation

$$s_n=\sin(\phi_{n+1}-\phi_n-\alpha)\ . \tag{16}$$

Then Eq. (7) can be written in terms of ϕ_n and s_n as

$$s_n-s_{n-1}=2\gamma\sin(2\phi_n)\ . \tag{17}$$

The variable ϕ is defined mod π and lies in the range $[0, \pi]$, while the variable s is restricted to lie in the range $[-1, +1]$ in order that the inverse sine be well defined. With these restrictions, Eqs. (16) and (17), which we rewrite here for convenience in the form

$$\phi_{n+1} = \phi_n + \alpha + \arcsin s_n \; ,$$
$$s_{n+1} = s_n + 2\gamma \sin(2\phi_{n+1}) \; , \tag{18}$$

define a mapping of a part of the surface of a cylinder onto itself. This mapping, $G(\phi_n, s_n) \rightarrow (\phi_{n+1}, s_{n+1})$, can be trivially shown to be area preserving. This map is in many respects similar to the Taylor-Chirikov map, yet significantly different from it.

Two-dimensional area-preserving mappings have been studied in different contexts and attention has mainly focused on the nature of the fixed points of the mapping and the nature of the curves left invariant by the mapping.[37–39] In this section we present two approaches to investigating the nature of the invariant curves of the mapping G. The first is an approximate analytical approach. The second is a numerical investigation which utilizes the fact that Eqs. (18) define a recursion relation in the pair of variables (ϕ_n, s_n).

Broadly speaking, an invariant curve of any area-preserving map may belong to one of the following classes: (a) it may be composed of a finite number, m, of discrete points (fixed point of G^m corresponding to a commensurate configuration of order m), (b) it may be a smooth, continuous curve, known as a Kolmogorov-Arnold-Moser (KAM) curve (corresponding to an incommensurate configuration), or (c) it may be a chaotic trajectory, the points of which form a Cantor set. There are fairly general theorems[27,29] which say that under certain circumstances (γ greater than some γ_c in our model) each KAM curve ceases to be smooth and continuous and disintegrates into a chaotic set of points. Aubry has speculated[26,27,29] that the existence of KAM curves in the mapping in some sense implies that the associated devil's staircase is incomplete and that when all of the KAM curves have disintegrated into chaotic trajectories, the devil's staircase becomes complete everywhere.

If $s(\phi)$ is the equation of an invariant curve, after one application of the transformation the point (ϕ, s) on this invariant curve is mapped into the point $(\tilde{\phi}(\phi,s), \tilde{s}(\phi,s))$. This new point must satisfy the same equation as the original point. This leads to a functional equation for $s(\phi)$:

$$s(\phi) + 2\gamma \sin 2[\phi + \alpha + \arcsin s(\phi)] = s[\phi + \alpha + \arcsin s(\phi)] \; . \tag{19}$$

Assuming γ to be small we may expand s as a power series in γ,

$$s(\phi) = \sum_{k=0}^{\infty} s_k(\phi) \gamma^k \; . \tag{20}$$

In what follows, the inverse sine proves rather awkward to handle. We have overcome this difficulty by using the small-argument power-series expansion for the inverse sine[40] and then successively retaining higher-order terms. Substituting Eq. (20) into Eq. (19) and equating coefficients of equal powers of γ on the two sides of the equation, we obtain, for the three lowest-order terms,

$$s_0 = \text{const} \; , \tag{21a}$$

$$s_1 = \frac{-1}{\sin\delta} \cos(2\phi + \delta) \; , \tag{21b}$$

$$s_2 = \frac{Z}{2\sin^2\delta \sin 2\delta} \cos(4\phi + 4) \; , \tag{21c}$$

where

$$\delta = \alpha + \arcsin s_0 \tag{21d}$$

and

$$Z = \frac{d}{dy} \sin^{-1} y \bigg|_{y=s_0} \; . \tag{21e}$$

The first-order term in Eq. (20) is small compared to the zeroth-order term unless s_0 lies in the "first-order dangerous bands" which are bands of width $\sim\gamma^{1/2}$ around the lines $s_0 = \pm\sin\alpha$. Likewise, the term proportional to γ^2 is small compared to the first-order term if s_0 lies outside both the first-order dangerous bands and the second-order dangerous bands, which are of width $\sim\gamma$ around the lines $s_0 = \pm\cos\alpha$. The extension to higher-order terms can be easily effected and higher-order dangerous bands arise. For small γ, most curves are straight lines with a slight modulation.

In order to investigate the nature of the invariant curves in the dangerous bands, we start with the simplest assumption that $|s|$ is small. Expanding both sides of Eq. (19) in powers of s and γ, we obtain, in the first approximation,

$$s(\phi) s'(\phi) = \gamma \sin\phi \; , \tag{22}$$

where the prime indicates differentiation with respect to the argument. The solution to this equation is

$$\tfrac{1}{2} s^2 = \gamma(C - \cos\phi) \; , \tag{23}$$

where C is a constant. For $C > 1$ the solution is a periodic curve, while for $-1 < C < 1$ the solution is a closed curve which degenerates into a point at $C = -1$. This point is also a fixed point of the mapping. The solution with $C = 1$ represents a separatrix joining two fixed points and separating regions of closed and open curves. This solution corresponds physically to a single kink in the system making a smooth transition between neighboring configurations represented by the fixed points joined by the separatrix. The results for the higher-order dangerous bands are similar. In the second-order bands we again have a system of closed and open periodic curves whose period is half that of the closed curves in the first-order bands. The whole picture then consists of bands of closed curves (bounded by separatrices) and periodic open curves, with higher-order bands (of decreasing width as the order increases) occupying the regions between the lower-order bands.

These results are valid only to the degree to which the power-series expansions are valid. Unfortunately, the series in Eq. (20) is only an asymptotic series which does not converge for any value of γ, and exponential devia-

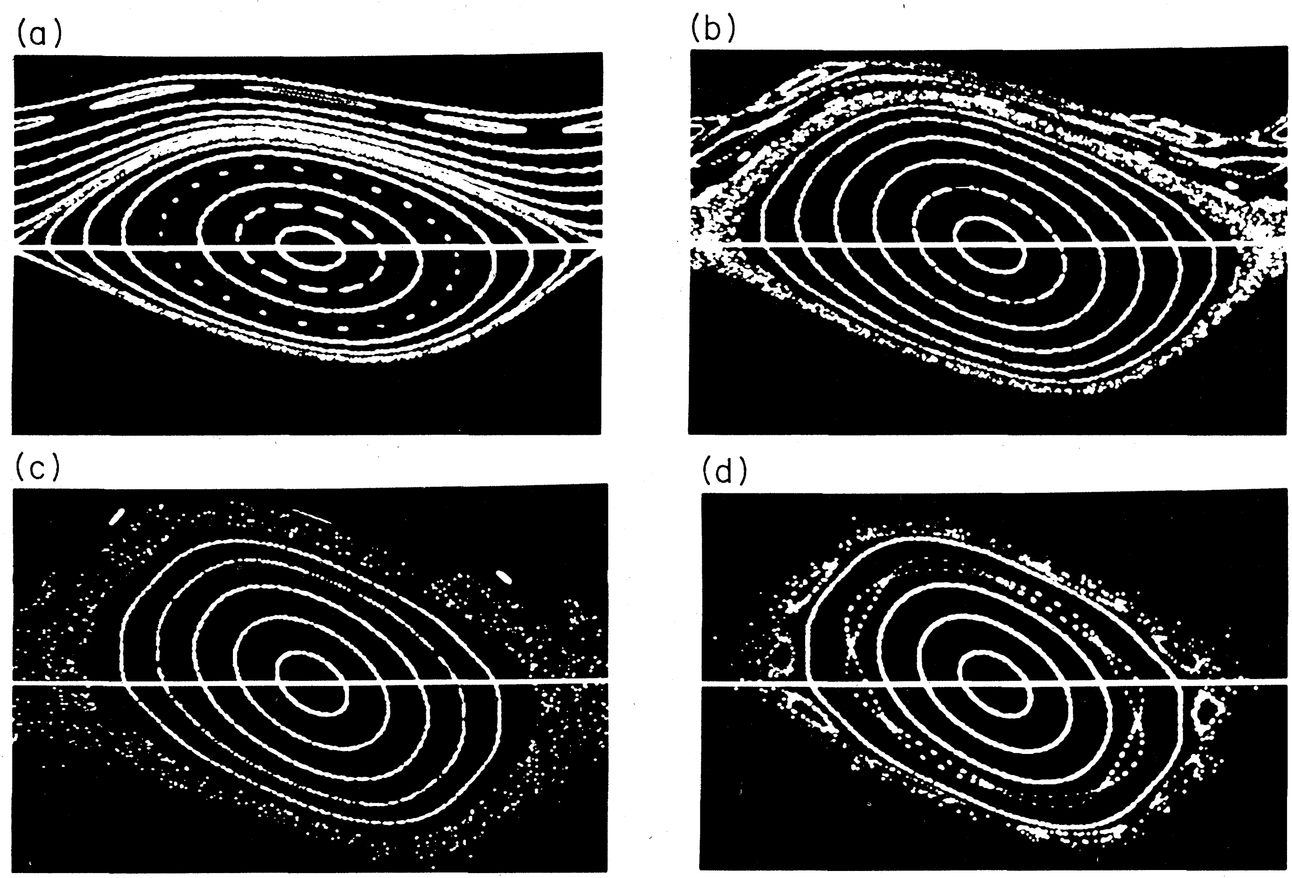

FIG. 9. Invariant trajectories of the mapping G at $\alpha=0$ and (a) $\gamma=0.0850$, (b) $\gamma=0.1400$, (c) $\gamma=0.1800$, and (d) $\gamma=0.19213$. The quantity ϕ increases from 0 to 2π along the abscissa while s varies from -1 to $+1$ along the ordinate.

tions from our results may be expected.[39] Another drawback of this approach is that it seems to indicate that the only fixed points of the transformation are fixed points of orders 2^n, since fixed points of any other orders do not appear in this treatment. That fixed points of other orders must exist is clear from the fact that commensurate phases of orders $m\neq 2^n$ exist, and these correspond to mth-order fixed points of the transformation. The existence of these other fixed points can also be seen clearly from the numerical work which we discuss next.

A second method of generating curves invariant under the mapping is to apply the mapping repeatedly to any point in the rectangle. Under such successive applications of the mapping, each point (ϕ,s) traces out a trajectory in the rectangle. Each such trajectory is, by the nature of its construction, invariant under the mapping, i.e., the points on each such trajectory map onto each other. This method of generating invariant curves shows up a number of different classes of invariant curves which cannot be found by the method described in the preceding paragraphs. In particular, interesting "chaotic" trajectories, which play a very important role in the analysis of the system, can be quite clearly seen.

Figure 9 shows sets of invariant curves obtained from the recursion relations represented by Eqs. (18). We have set the parameter $\alpha=0$ for all the curves (a nonzero value of α does not change the nature of the trajectories in any significant way) and all the figures have the same starting points, while γ increases as shown from 0.0850 in Fig. 9(a) to 0.192 13 in Fig. 9(d). The general agreement between the predictions of the analytical and numerical calculations is clear. One can plainly see the bands (some of them quite distorted because γ is not small) of closed curves and the separatrices that separate them from the open curves. The disintegration of what appear to be smooth continuous curves into chaotic ones and the increase in the region occupied by these chaotic curves can also be seen. From these results we are led to believe that KAM curves do indeed exist in this mapping for $\gamma>0$, and that these KAM curves disintegrate into chaotic curves above some value γ_c. This in turn implies that the devil's staircase referred to in the preceding sections is incomplete for $\gamma<\gamma_c$ and complete for $\gamma>\gamma_c$. While it has been possible[41] in the case of the discrete sine-Gordon system to determine the value of "the winding number" at which the last of the KAM curves of the Taylor-Chirikov map disintegrates into a chaotic trajectory, it has, unfortunately, not yet been possible to do this for our map.

VI. DISCUSSION

We have presented here a phenomenological model that might be useful in understanding the incommensurate-commensurate phase transitions that occur in different types of materials, principally in SDW and CDW systems and in certain helical macromolecular systems such as PTFE. Although the study of the model is far from complete and a large number of questions remain unanswered, a great deal has been learned about this model. In our study of the model at $T=0$, we have shown strong evidence that the phase diagram of this model is composed of an infinite number of commensurate phases. We have also shown that the variation of the mean angle between nearest-neighbor arrows with the degree of natural cantedness of the system is of the form of a devil's staircase. By studying the behavior of the system at finite temperatures, we have shown that kinks play an important role in shaping the phase diagram of the system. Finally, we have found an area-preserving map associated with this model and have studied the invariant curves of this map using analytical and numerical techniques. We have seen evidence for the existence of KAM curves and that each KAM curve disintegrates into a chaotic set of points at a critical value of the parameter γ. From this we have concluded that the devil's staircase is incomplete below a certain critical value of γ and is complete for all $\gamma > \gamma_c$.

A number of interesting questions remain unanswered about this model. We have restricted our attention to the convex regions of the nearest-neighbor interaction potential, and have shown that in certain regions of the phase diagram the ground state must remain in the convex regions. We have not yet been able to make any such claim about the entire α-γ plane, and it is possible that in certain regions of the phase diagram the nonconvex regions of the potential may actually be preferred. It is conceivable that the model might show unexpected and interesting behavior if the nonconvex regions were accessible and even preferable. This possibility should be explored. It would, of course, be desirable to put many of our results on a firmer mathematical footing by, for instance, obtaining a rigorous proof that there is indeed a true devil's staircase associated with this model. A more thorough and complete investigation into the completeness of the devil's staircase is also important, as this has serious implications for the nature of the experimentally observed transitions. Another question that might profitably be addressed is the question of universality in the transitions associated with the devil's staircase. There is a hint of scale invariance in the nature of the devil's staircase, where between any two commensurate phases there is an infinite number of commensurate phases so that any part of the staircase looks rather like the whole. Shenker and Kadanoff,[41] and recently Jensen, Bak, and Bohr,[42] have found that various features of the destruction of the KAM curves in the Frenkel-Kontorova model seem to be universal and show scale invariance. The destruction of the KAM curves in our model should be carefully examined with a view to answering questions about scale invariance and universality.

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*Present address: Department of Physics, West Virginia University, Morgantown, WV 26506.

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