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Frenkel–Kontorova Model with Alternant Coupling Potential*

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Abstract *We have studied a modified Frenkel–Kontorova (FK) model with alternant coupling potential. From it, we obtain a coupling conservative map, it shows that the gold-mean number is not the last broken winding number, and the broken critical value is varied with the variance of strength of spire. The phase diagram becomes asymmetric in a period. The Devil's staircase and generalized dimension are different from those of the standard FK model.*

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Key words: Devil's staircase, Frenkel–Kontorova (FK) model, alternant coupling potential

1 Introduction and the Model with Alternant Coupling Potential

Commensurate-incommensurate phase transition has been observed in many condensed matter systems, such as charge-density waves, magnetic spirals and adsorbed monolayer. A simple one-dimensional model, the Frenkel–Kontorova (FK) model, has been widely used to study this transition.[1−8]

In the standard FK model, the coupling potential between atoms is uniform quadratic. But in many realistic systems, it is nonuniform.[9,10] In this paper, we study a more generalized FK model with an alternant coupling potential. The coupling potential W among three neighbor atoms is given by

$$W(x_{i+1},x_i,x_{i-1}) = \frac{1}{2}k_1\Big(x_{i+1}-x_i-\frac{\mu_1}{k_1}\Big)^2 + \frac{1}{2}k_2\Big(x_i-x_{i-1}-\frac{\mu_2}{k_2}\Big)^2\,, \tag{1}$$

where, we give $\mu_1=\mu_2=\mu$ and two kinds of appropriate original length of the springs μ/k_1 and μ/k_2, and k_1, k_2 are the coefficients of elasticity of the springs.[11−13]

If we consider an external cosine potential, the Hamiltonian for the generalized FK model with an alternant coupling potential can be written as

$$H = \sum_{i=\mathrm{odd}}\Big\{\frac{1}{2}k_1\Big(x_{i+1}-x_i-\frac{\mu}{k_1}\Big)^2 + \frac{1}{2}k_2\Big(x_i-x_{i-1}-\frac{\mu}{k_2}\Big)^2 + \frac{k}{(2\pi)^2}[1-\cos(2\pi x_i)] + \frac{k}{(2\pi)^2}[1-\cos(2\pi x_{i-1})]\Big\}. \tag{2}$$

where k is the strength of the external potential.

2 Ground State

Let ω denote the mean distance between successive atoms

$$\omega = \lim_{n\to\infty}\frac{x_n-x_0}{n}\,. \tag{3}$$

Considering a commensurate structure with winding number $\omega=p/q$, the initial positions of q atoms are set up in equal-space array,

$$x_i(0) = i\frac{p}{q}+\alpha\,,\qquad i=1,2,\ldots,q\,, \tag{4}$$

where the phase α satisfies $m_i\le 2(i\omega+\alpha)\le m_i+1$ and $m_i=[2x_i]$.

We can solve the q differential equations

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = f_i = -\frac{\partial H}{\partial x_i}\,,\qquad i=1,2,\ldots,q\,. \tag{5}$$

A periodic condition

$$x_0 = x_q - p\,,\qquad x_{q+i} = x_i + p \tag{6}$$

is imposed.

We use the gradient method to calculate the periodic ground state to 10^{-7} accuracy, then improve the accuracy to 10^{-14} by Newton method.

Because the ground state is only metastable configuration for very small k value. For a given ω, we start with $k=0$, then next k with a small increment in k.

3 Map and Critical Point

The equilibrium configuration of the Hamiltonian (2) can be expressed as a map. By the equilibrium condition,

$$-\frac{\partial H}{\partial x_i} = 0\,. \tag{7}$$

Define the conjugate variable P_i, $P_{i+1}=x_{i+1}-x_i$, the condition (7) can be written as

$$k_1P_{i+1}-k_2P_i-\frac{k}{2\pi}\sin(2\pi x_i)=0\,,\qquad x_{i+1}=P_{i+1}+x_i\,,\qquad i=\mathrm{odd}\,, \tag{8}$$

$$k_2P_i-k_1P_{i-1}-\frac{k}{2\pi}\sin(2\pi x_{i-1})=0\,,\qquad x_i=P_i+x_{i-1}\,,\qquad i=\mathrm{odd}\,. \tag{9}$$

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The Jacobis of Eqs (9) and (10) are k_2/k_1 and k_1/k_2. The continuing iteration of two maps is an area-preserving map. But each of them is dissipative. We can write them in area-preserving style,

$$P_{i+1} = P_{i-1} + \frac{1}{k_1}\frac{k}{2\pi}\sin(2\pi x_{i-1}) + \frac{1}{k_1}\frac{k}{2\pi} \times \sin\Big(2\pi\Big(\frac{k_1}{k_2}P_{i-1} + \frac{k}{2\pi}\frac{1}{k_2}\sin(2\pi x_{i-1}) + x_{i-1}\Big)\Big),$$

$$x_{i+1} = P_{i+1} + \frac{k_1}{k_2}P_{i-1} + \frac{k}{2\pi}\frac{1}{k_2}\sin(2\pi x_{i-1}) + x_{i-1}\,. \quad (10)$$

To study the critical behavior, finding critical point is very important. At this point, we first find the point corresponding to the gold-mean winding number breaking up. We will use Green's residue criterion to determine the critical point.[12] The Green's residue criterion states

$$\lim_{i\to\infty} R_i^e(k) = \begin{cases} 0^+\,, & k < k_c\,, \\ a\,, & k = k_c\,, \\ \infty\,, & k > k_c\,, \end{cases}$$

$$\lim_{i\to\infty} R_i^h(k) = \begin{cases} 0^-\,, & k < k_c\,, \\ -b\,, & k = k_c\,, \\ -\infty\,, & k > k_c\,, \end{cases}$$

where $R_i^e(k)$ and $R_i^h(k)$ are the residues of elliptic and hyperbolic orbits, and a, b are positive constants less than unity. The residue R is defined via the Jacobian matrix M of the linearized maps (9) and (10),

$$\begin{pmatrix} \delta P_{i+1} \\ \delta x_{i+1} \end{pmatrix} = M_i M_{i-1} \begin{pmatrix} \delta P_{i-1} \\ \delta x_{i-1} \end{pmatrix},$$

where

$$M_i = \begin{pmatrix} 1 + \frac{k}{k_1}\cos(2\pi x_i) & \frac{k}{k_1}\cos(2\pi x_i) \\ \frac{k_2}{k_1} & \frac{k_2}{k_1} \end{pmatrix},$$

$$M_{i-1} = \begin{pmatrix} 1 + \frac{k}{k_2}\cos(2\pi x_{i-1}) & \frac{k}{k_2}\cos(2\pi x_{i-1}) \\ \frac{k_1}{k_2} & \frac{k_1}{k_2} \end{pmatrix},$$

$$M = \prod_{i=1}^{q} M_i\,, \qquad R = \frac{1}{4}(2 - \mathrm{Tr}\,(M))\,.$$

We give out the critical point corresponding to gold-mean winding number for different k_1 and k_2 in Fig. 1. Here $k_1 = 2 - k_2$. We find that the critical point varies with k_1 and k_2. In $k_2 \in [0.2, 1.0]$, there are two tops and $k_1 = k_2$ is the hardest.

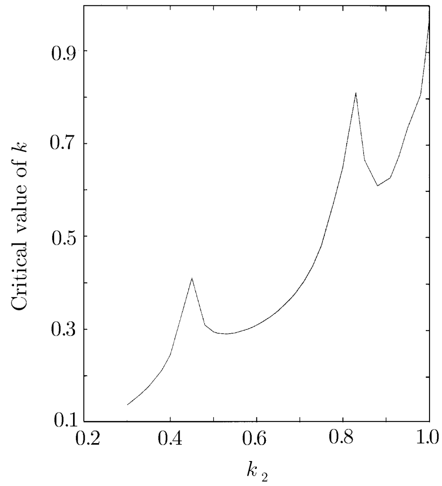

Fig. 1 The critical value vs. k_2.

For $k_1 = 0.5$, $k_2 = 1.5$, we give out Fig. 2, which corresponds to the gold-mean winding number and has the critical value $\lambda = 0.2953$. Because there are many KAM orbits, the gold-mean winding number is not the last broken point in this case. Then, we find that the last broken point's critical value is $k_c = 0.74$, as shown in Fig. 3. The corresponding winding number is $\omega_{\rm last} = 3979/4360$.

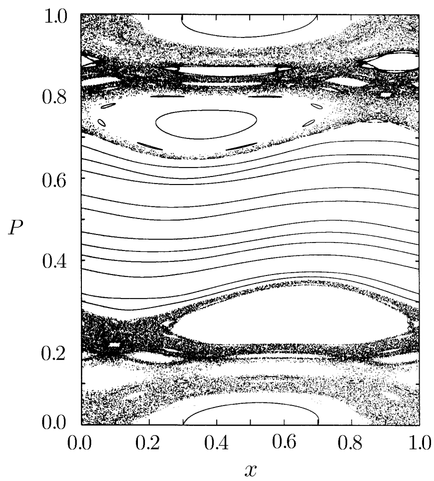

Fig. 2 The phase figure corresponding to the golden winding number.

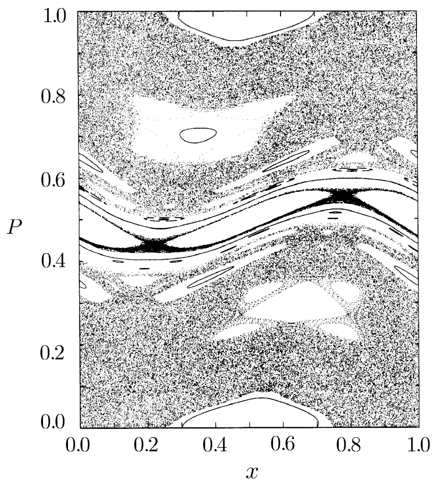

Fig. 3 The phase figure corresponding to the last broken KAM curve.

4 Phase Diagram

In this model, there are two parameters: the equilibrium lattice constant of the free chain μ and the strength of the external potential k. They form a two-dimensional parameter space. It has been shown that the phase diagram exhibits a tongue for each rational in the winding number interval $\omega \in [0, 2]$.

We take advantage of the Faray tree construction to study the phase diagram.[13] The most effective way to construct a phase diagram is to local the boundaries of commensurate states for a given commensurate state $\omega = p/q$, the other commensurate state $\bar{\omega} = \bar{p}/\bar{q}$ is infinitely close to ω, $\bar{q} \gg q$. If $\bar{\omega}$ is enough high order, their energies should be also infinitely close.

We rewrite the Hamiltonian as

$$H = \sum_{i=\text{odd}} \Big[\frac{1}{2}k_1 x_{i+1}^2 + \frac{1}{2}k_1 x_i^2 + \frac{1}{2}k_2 x_i^2 + \frac{1}{2}k_2 x_{i-1}^2 - \frac{k}{(2\pi)^2}\cos(2\pi x_i) - \frac{k}{(2\pi)^2}\cos(2\pi x_{i-1}) - (k_1 x_{i+1}x_i + k_2 x_i x_{i-1})\Big] - \mu p + \frac{q}{4}\Big(\frac{1}{k_1} + \frac{1}{k_2}\Big)\mu^2 \,. \quad (11)$$

A boundary μ_B of commensurate $\omega = p/q$ at a given K is determined by the equation

$$H(\omega, k, \mu_B) = H(\bar{\omega}, k, \mu_B) \,. \quad (12)$$

We have used the expression (12) to calculate the phase diagram of model (3). Figure 4 is the phase diagram at $k_1 = 0.5$, $k_2 = 1.5$. It shows that the phase diagram is asymmetric at the interval $\omega \in [0, 2]$.

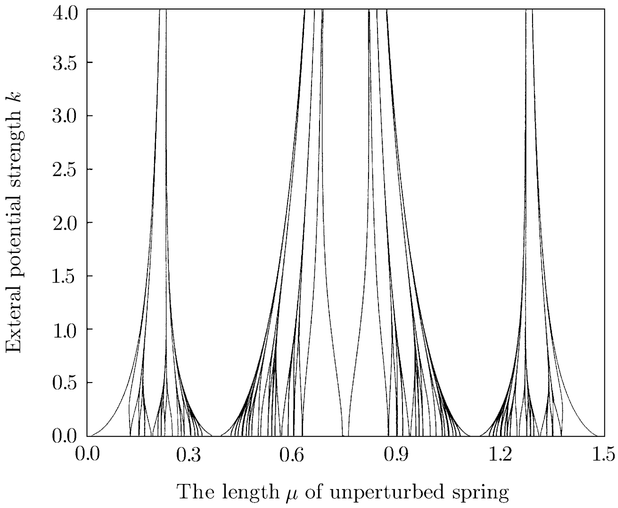

Fig. 4 The tongue figure.

5 Devil's Staircase and Dimension

It has been shown that on or above the critical value k_c, the frequency ratio ω as a function of the parameter μ forms a complete Devil's staircase (DS) as shown in Fig. 5. This function contains only steps. Each of them represents a commensurate state. We study the Devil's staircase at the critical golden-mean value $k_c(\omega_G)$. Figure 5 shows the influence of the alternant coupling potential, compared to the staircase of the standard FK model, the steps move to the left and right sides. The complementary set of a complete devil's staircase is a fractal with zero measure. By defining a fractal measure on the fractal, we can study the multifractal properties. We use ϵ_i to denote the width of the i-th piece, m_i denotes the fractal measure defined as the difference of the winding numbers of two neighboring steps,

$$m_i = \omega_{i+1} - \omega_i \,, \qquad i = 1, 2, \ldots, 2^{n-1} \,, \quad (13)$$

they satisfy the condition

$$\sum_i m_i = 1 \,. \quad (14)$$

The partition function in the n-th Farey generation is

$$\Gamma^{(n)}(q, \tau) = \sum_{i=1}^{2^{n-1}} \frac{m_i^q}{\epsilon_i^\tau} \,. \quad (15)$$

We can obtain the function $\tau(q)$ by equating the above equation to a finite constant C. Here, we choose $C = 1$, then τ is defined by

$$\sum_{i=1}^{2^{n-1}} \frac{m_i^q}{\epsilon_i^\tau} = 1 \,, \quad (16)$$

α is defined as

$$\alpha(q) = \Big(\sum_{i=1}^{2^{n-1}} \frac{m_i^q}{\epsilon_i^\tau} \ln m_i\Big) \Big/ \Big(\sum_{i=1}^{2^{n-1}} \frac{m_i^q}{\epsilon_i^\tau} \ln \epsilon_i\Big). \quad (17)$$

The singularity spectrum $f(\alpha)$ and the generalized dimension D_q can be calculated,

$$f(\alpha) = q\alpha(q) - \tau(q) \,, \qquad D_q = \frac{\tau(q)}{q-1} \,. \quad (18)$$

The numerical results are shown in Figs 6 and 7. The peak of the singularity spectrum curve corresponds to $q = 0$, $\alpha_0 = \alpha_{\max}$, and the corresponding generalized dimension is $D_0 = 0.812$ in this case, $k_1 = 1.5$, $k_2 = 0.5$. It is different from the standard FK model case.

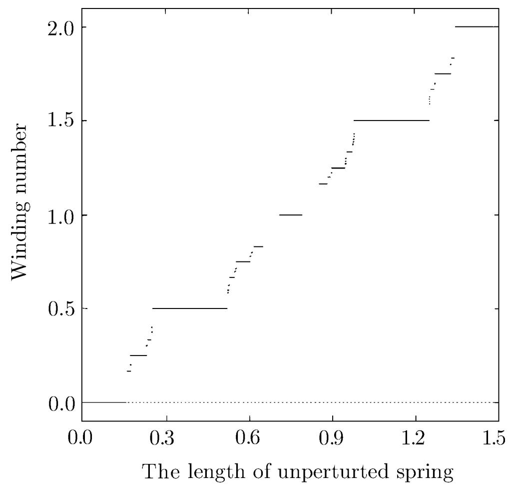

Fig. 5 The Devil's staircase.

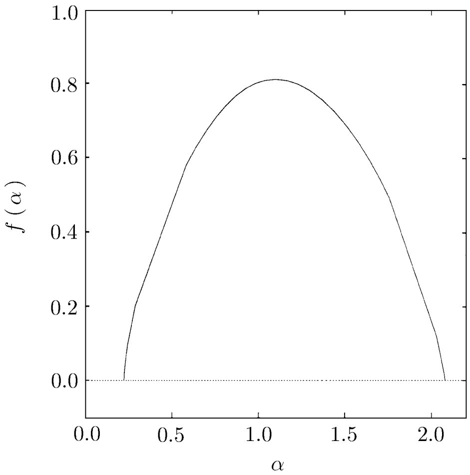

Fig. 6 Singularity spectrum $f(\alpha)$ of the complete Devil's staircase at $k_1 = 1.5$, $k_2 = 0.5$.

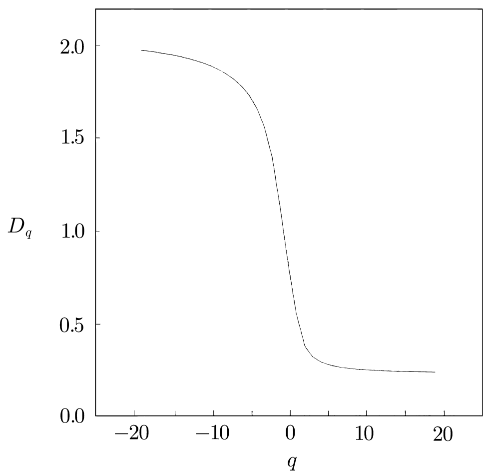

Fig. 7 Generalized dimension D_q of the complete Devil's staircase at $k_1 = 1.5$, $k_2 = 0.5$.

6 Discussions and Conclusions

We have studied a strongly nonlinear system: the FK model with an alternant coupling potential. A number of new features appear because of this potential. The phase diagrams become asymmetric. The critical values become small when the difference of coefficient of the elasticity increases. In particular, the generalized dimension varies as the elastic coefficient. The coupling potential destroys the internal symmetry of the FK model.

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