The static properties of multi-chain Frenkel–Kontorova model: ground state and static friction

Li Haibin *, Zhao Hong, Wang Yinghai

Department of Physics, Lanzhou University, Lanzhou 730000, China

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Abstract

The static properties of the multi-chain Frenkel–Kontorova model are studied numerically. In the case of incommensurate structure, the transition by breaking of analyticity appears in each chain. A new hull function $h(x)$, which also shows the transition by breaking of analyticity, is defined. The static friction (depinning force) depends strongly on the strength of the substrate potential, the number of chains and the strength of the interaction between chains. © 2002 Elsevier Science B.V. All rights reserved.

1. Introduction

The Frenkel–Kontorova model [1] is a simple one-dimensional model used to describe nonlinear phenomena such as dislocation dynamics, charge-density wave [2], ferroelectric domain wall [3] and commensurate–incommensurate transition. In general, the F–K model consists of a chain of atoms coupled by the harmonic nearest neighbor interaction. The chain is subjected to an external sinusoidal potential. Studies on the incommensurate structure of the ground state of F–K [4] have shown an phase transition called the breaking of analyticity. This transition is determined by the amplitude of the substrate potential. Extensive studies on the ground state of the F–K model with other kinds of interatomic force have presented a similar phase transition [5,6].

The F–K model has also been used as a simple friction model which describes a atomic monolayer of a soft body sliding on a flat surface [7]. In recent years, the study of friction has been attracting much attention in physics. It is well-known that the three laws of friction force hold well in a usual situation [8]:

(1) The friction force is independent of the apparent area.
(2) The friction force is proportional to the normal load.
(3) The kinetic friction force does not depend on the velocity.

Recently, the development of new technology has made it possible to study friction at microscopic level [9–11]. The friction process range various in spatial and temporal scales from microscopic to macroscopic [12]. Interest in the nature of friction has been growing and many theoretical treatments have presented a variety of characteristics of friction [13–20].
Except the F–K model, several simple models have been introduced in the hope of yielding the applicable analytical results. These models include many layer model with harmonic interaction \[21,22\], the Frenkel–Kontorova–Tomlinson model \[23\], a single layer model with harmonic interaction \[24\] and other complicated nonlinear models \[25–30\].

In this Letter, the F–K model is extended into a multi-chain F–K model in which the chains are coupled via a harmonic spring. The ground state of the quasi-two-dimensional multi-chain F–K model is studied and new static and dynamic characteristics are observed in the presence of an external potential on the boundary. The different behaviors of each chain in the multi-chain F–K model during the transition of analytic breaking are studied. As a model to study dry friction, the multi-chain F–K model describes the volume effect on the static friction force which has been defined as the depinning force in the F–K model. The zero friction sliding and power law are the dynamic characteristics of the F–K model in the incommensurate case. When the number of chains and coupling constant vary, the static friction exhibits interesting behaviors.

2. Model

As discussed in the introduction, our main aim in this Letter is to consider the static properties of the multi-chain F–K model with a quasi-two-dimensional structure. We extend the original F–K model to the multi-chain F–K model (see Fig. 1). This new model consists of many chains and each chain is made up of atoms with the harmonic nearest neighbor interaction. The chains are also coupled to each other by the harmonic nearest neighbor interaction. It should be pointed out that only the first chain is situated in the sinusoidal potential which defines a hard surface. In studying friction, the sliding body is no longer monolayer but multi-layer. The free energy of the multi-chain model in dimensionless form is

$$
\Psi(u_{i,j}) = \sum_{j=1}^{M} \sum_{i=1}^{N} \frac{1}{2} \left[ (u_{i+1,j} - u_{i,j})^2 + \gamma (u_{i,j} - u_{i,j-1})^2 \right] + \frac{k}{2\pi} \sum_{i}^{N} \cos(2\pi u_{i,1}/a),
$$

(1)

where \(u_{i,j}\) is the position of the atom, the parameter \(k\) is the amplitude of the external periodic potential with period \(a\). The second term on the left-hand side of Eq. (1) is the coupled term between the neighboring chains and \(\gamma\) is the elastic constant. Note that the index \(i, j\) label the particle within a chain with integer \(i (i = 1, \ldots, N)\) and the chain with integer \(j (j = 1, \ldots, M)\), so that the system consists of a total number of \(N \times M\) atoms.

The periodic boundary conditions are taken in each chain in the direction labeled by the index \(i\),

$$
u_{i+N,j} = u_{i,j}.
$$

(2)

In the direction labeled by \(j\), the boundary condition is chosen as free condition, which means that the lower most chain interacts with the external potential and the upper most chain interacts only with the chain beside it. To calculate the ground state of the multi-chain F–K model and study the static and quasistatic (depinning force) dynamic properties, we use the ‘gradient method’ \[4\] as our computer simulation method.

3. Ground state

In this section, we investigate the ground state of the multi-chain F–K model. The ground state is the solution of the following equation \[4\]

$$
\frac{\partial \Psi(u_{i,j})}{u_{i,j}} = 0.
$$

(3)
Because the atom moves along the direction labeled by \( i \), the above equation becomes

\[
\sum_{j=2}^{M-1} (u_{i+1,j} + u_{i-1,j} - 2u_{i,j}) + \gamma(u_{i,j+1} + u_{i,j-1} - 2u_{i,j}) = 0,
\]

\[
u_{i+1,M} + u_{i-1,M} - 2u_{i,M} + \gamma(u_{i,M-1} - u_{i,M}) = 0,
\]

\[
u_{i+1,1} + u_{i-1,1} - 2u_{i,1} + \gamma(u_{i,2} - u_{i,1}) - \frac{k}{2\pi} \sin(2\pi u_{i,1}/a) = 0.
\]

(4)

Let \( d \) denote the atomic mean distance in the chain labeled by \( i \),

\[
d = \lim_{n,n' \to \infty} \frac{u_{n,j} - u_{n',j}}{n - n'} \quad (j = 1, 2, \ldots, M).
\]

(5)

In the absence of the periodic potential, the equilibrium position of the particle satisfying the boundary condition can be given by

\[
u_{i,j} = id + \alpha,
\]

(6)

where \( \alpha \) is an arbitrary phase.

The ground state of multi-chain F–K model is a commensurate structure if the ratio \( d/a \) is rational. If \( d/a \) is irrational, the ground state is an incommensurate structure which can be described by a hull function as follows

\[
u_{i,j} = f(id + \alpha) = id + \alpha + g(id + \alpha),
\]

(7)

where \( g(x) \) is a periodic function with the same period \( \alpha \) as the external potential.

The definition of the ground state, the atomic mean distance and hull function are used to deal with the original F–K model [4]. The transition in the ground state of the F–K model takes place in the incommensurate state with an irrational \( d/a \) ratio. If the amplitude of the external potential \( k \) is small, the hull function \( f(x) \) is an analytic function, but when \( k \) is large enough, \( f(x) \) varies discontinuously and becomes a sum of step functions. This transition by the breaking of analyticity was also found to occur at a well-defined value of \( k \) (\( k_c = 0.9716 \)). On the other hand, Eq. (3) of the original F–K model can be deduced to an area-preserving map (the well-known standard map) by variable transformation. The transition by breaking of analyticity of the hull function \( f(x) \) describing the ground state of F–K model and the change to stochasticity in the standard map are connected because the transition in the ground state of the F–K model corresponds to the disappearance of a Kolmogorov–Arnold–Moser (KAM) torus.

When the ground state is commensurate, the hull function (7) is trivial and cannot describe the configuration of the ground state of the F–K model. So, our numerical calculation firstly gives the exact position of each particle and shows the configuration of the multi-chain F–K model with different \( d/a \) ratios.

When \( d/a = 1 \), we find that each chain has the same configuration, which means the coordinates of the atoms with the same index \( i \) are equal to each other

\[
u_{i,j} = u_{i,j'} \quad (j \neq j').
\]

(8)

and all the chains act as a whole. The motion of the model can then be treated as the motion of one chain.

When \( d/a = \frac{1}{T} \) (\( T = 2, 3, 4, \ldots \)), the positions of atoms in a chain are not the same as their counterparts in the neighboring chain or other chains at each site. They are only equal at periodic sites

\[
u_{i,j} = u_{i,j'} \quad (j \neq j', i = nT, n = 1, 2, 3, \ldots).
\]

(9)

For example, \( a = \frac{1}{2} \), \( u_{2n,j} = u_{2n,j'} \) (\( j \neq j', n = 1, 2, 3, \ldots \)). So the configuration of chains are locally different, but equivalent on the whole. When the incommensurability of \( d/a \) increases, the local difference will become global as discussed below.

Recall that when \( d/a \) is irrational, the hull function \( f(x) \) is applied to describe the atomic configuration of the F–K model. Considering the simplicity in our extension of the F–K model, we still use the above definitions of the atomic mean distance and hull function for the multi-chain F–K model. If the number of chains equals one, the above definitions refers their original meaning.

Taking into account the fact that the multi-chain F–K model has many layers, we first rewrite Eq. (7) as

\[
u_{i,j} = f_j(id + \alpha_j) = id + \alpha_j + g_j(id + \alpha_j).
\]

(10)

\( \alpha_j \) is an arbitrary phase difference in the chain labeled by \( j \). Fig. 2a,b show the hull function of numerically calculated ground state of the two-chain F–K model with coupling constant \( \gamma = 0.5 \) for an incommensurate value of \( d/a, 233/377 \), an approximator of the golden mean \((\sqrt{5} - 1)/2\). It is clearly seen
in Fig. 2 that the profile of the hull function is similar to that of the original F–K model. The phenomenon of analytic breaking is also a property of the hull function. When $k < k_c$, the hull function is continuous, if $k > k_c$, the hull function becomes a step function. This phenomenon occurs in the hull function of each chain. We check the hull function of each chain and find the same analytic breaking transition when $k$ increases. Moreover, we also find the critical values $k_c$ of all hull functions $f_j(id + \alpha_j)$ to be identical. In other words, if $k$ increases beyond a certain value $k_c$, then the hull function related to each chain undergoes the same analytic breaking transition. This is a global change in the multi-chain F–K model.

On the other hand, we note that the hull function of each chain is different in our detailed simulation. This indicates that the ground state is defective in the region $k > k_c$, but has different defective forms for each chain because the ground state configuration of each chain is different. The defective state refers to the energy function (1) with a local minimum corresponding to the metastable state. On the contrary, if $k < k_c$, the energy has only one minimum. To show the differences between the two hull functions $f_j(x)$, we define a function $h(x)$ to describe the numerical result as follows:

$$h_{i,j}(x) = f_i(x) - f_j(x) \quad (i \neq j).$$

Fig. 3a,b present the new hull function $h(x) = h_{2,1}(x)$ which describes the configuration difference between the first and second chain of the two-chain F–K model. It is revealed that $h(x)$ is not trivial, but exhibits a sinusoidal behavior. This suggests that the different chains have different configurations in the incommensurate ground state. The existence of the potential adjusts the configuration of the F–K model. Fig. 3 also shows that $h(x)$ has a transition when $k$ increases. It can be seen that there exists a critical value, $k'_c$. If $k < k'_c$, $h(x)$ is continuously analytic; if $k > k'_c$, the function $h(x)$ becomes a step function which varies discontinuously and the analyticity of $h(x)$ breaks. The configuration difference function $h(x)$, as well as $f(x)$, undergoes the phase transition. Furthermore, we calculate the precise value of $k'_c$ and find that it equals that of $f(x)$, i.e., $k_c = k'_c$.

The calculation of $h(x)$ in many chains model ($M = 3, 4, 5, \ldots$) shows that $h(x)$ for arbitrary two hull function $f_j(x)$ has the same form as in Fig. 3 and shows the same transition of analytic breaking.

Another interesting feature of the analytic breaking transition is that the critical value at which the
The hull function \( h(x) = f_2(x) - f_1(x) \) of the two-chain F–K model at different \( k \). (a) \( k = 1.0 \), (b) \( k = 2.0 \).

transition takes place in the multi-chain F–K model is larger than that of the original F–K model \((k_c = 0.9716)\). Further detailed calculation shows that the critical value of \( k \) varies in the multi-chain case with the variation of the number of chains and the strength of interaction between chains. The possible explanation for this result is that the more chains introduced into the F–K model will strengthen the stability of the structure (see Fig. 1). The interaction with the substrate potential will adjust the atomic displacement. The change in the configuration of a chain far from the potential is much less than that of a chain near the potential. To verify our point, we calculate \( k_c \) of the multi-chain F–K model \((M = 3, 4, 5, \ldots)\) with different interacting constants \( \gamma = 1.0, 0.5, 0.1 \) as shown partly in Fig. 4. It is obvious that the critical value \( k_c \) increases as the number of chains increases for the same \( \gamma \). It is also clear in this figure that when the number of chains increases, the growth of \( k_c \) is consistent with the exponential growth and \( k_c \) will tend to a finite value when the number of chains is large enough. In our numerical simulation, this tendency keeps on even for \( M = 15 \). On the other hand, for fixed number of chains \( M \), if the coupling constant \( \gamma \) increases, \( k_c \) increases as expected.

In summary, in the incommensurate case of the multi-chain F–K model, the analytic phase and analytic breaking phase consist of an assembly of configurations which shows a structural phase transition when \( k \) increases beyond a critical value \( k_c \). When the
number of chains is large enough, $k_c$ will converge into a finite value.

4. Static friction (depinning force)

The depinning force defined in the F–K model is a force applied to each atom of the chain. The stationary equation of the system becomes $F = -\frac{\partial^{2}\Psi}{\partial u_{i}^{2}}$. In the case of an irrational $d/a$ ratio, the ground state of the F–K model can be shifted by an infinitesimally small force when the amplitude of the periodic potential is below the critical value $k_c$, which means the chain is not locked to the lattice. On the contrary, if $k$ is greater than $k_c$, a finite force $F_c$ is needed to shift the chain. The chain will be kept on the lattice by the periodic potential if the force does not reach $F_c$.

When $k > k_c$, $F_c$ behaves as:

$$F_c(k) \propto (k - k_c)^\phi,$$  \hspace{1cm} (12)

$\phi$ is about 3.0 [4], which scales the dynamical behavior around the critical value $k_c$.

We continue to use the above definition of the depinning force for the multi-chain F–K model. The direction of the driving force is parallel to the direction labeled by the index $i$, the stationary equation is

$$F = -\frac{\partial^{2}\Psi}{\partial u_{i}^{2}},$$

$$F = (u_{i+1,M} + u_{i-1,M} - 2u_{i,M})$$

$$-\gamma(u_{i,M-1} - u_{i,M}) = 0,$$

$$F = (u_{i+1,j} + u_{i-1,j} - 2u_{i,j})$$

$$-\gamma(u_{i,j+1} + u_{i,j-1} - 2u_{i,j}) = 0,$$

$$F = (u_{i+1,1} + u_{i-1,1} - 2u_{i,1})$$

$$-\gamma(u_{i,2} - 2u_{i,1}) - \frac{k}{2\pi}\sin(2\pi u_{i,1}/a) = 0. \hspace{1cm} (13)$$

Eq. (13) determines the metastable state of the multi-chain F–K model. The depinning force $F$ of the two-chain F–K model is plotted in Fig. 5 as a function of $k$ with different $\gamma$. For a certain $\gamma$, there exists a $k_c$ in the variation of $k$, which shows a transition from nonfriction sliding to finite friction sliding. On the other hand, $k_c$ becomes large with increasing $\gamma$. Around each $k_c$, $F$ behaves as the power law form (12), but here $\phi$ is about 2.5.

In general, the static friction is not uniquely defined. The static friction depends on the internal state of the real contact area on the sliding surfaces and on the history of the friction system [31]. As we start with a metastable state and increase $F$ slowly, the state follows $F$ adiabatically until a certain value is reached at which the system depins locally and some degrees of freedom start to move. During the process of slowly increasing the driving force $F$, the system will follow a sequence of depinning events after which it locally relaxes into another pinned state. Eventually the system globally depins.

Applied to friction, the above definition is independent of the history of the friction system. The introduction of multi chains aims at understanding the effect of volume on static friction. The static friction force $F_s$ can be defined as the smallest driving force that phenomenologically initiates sliding. It corresponds to the depinning force in the F–K model. Therefore, any other force below $F_s$ does not generate a relative motion on the surface. The static force is also the force by which the system depins from metastable to unstable state.

We numerically calculate the static friction force $F_s$ (depinning force) for rational and irrational values of $d/a$. We note that the maximal static friction $F_s$ is monotonically increasing as a function of $k$. In the commensurate case, $k_c$ is zero. On the contrary, in the incommensurate case, $k_c$ has a finite value. If $k < k_c$, the static friction force $F_s$ is exactly zero because in
this region the hull function \( f(x) \) is analytic. This makes it possible for atoms to slide smoothly over the corrugated surface modeled as substrate potential. The static friction force and the breaking of analyticity appear together. Fig. 6 shows \( F_s \) for a sequences for rational values of \( d/a \) which approach the golden mean \((\sqrt{5} - 1)/2\). The curve sequences converges to a golden mean curve with a singularity at \( k_c \).

As the multi-chain F–K model has many layers, we can investigate the volume and structure effect on the static friction in the incommensurate case. The number of chains represents the volume effect and the coupling constant between the chains describes the structure effect. Two points are clear in Fig. 5. First, for a certain \( \gamma \), the increasing amplitude of the potential \( k \), which describes the roughness of the contact area, does not change the frictionless motion of the model when \( k < k_c \), but if \( k > k_c \), the static friction force will increase as \( k \) increases. Second, the strength of the coupling constant between chains is important to the static friction. \( \gamma \) can be treated as a parameter to measure hardness, which signifies the degree of interaction between neighboring chains. In Fig. 5, for a certain \( k \) beyond \( k_c \), the static force \( F_s \) becomes small as \( \gamma \) increases, which indicates that a harder body slides easier than softer one. Furthermore, we calculate the \( F_s \) of the many-chain case and find the result to be similar to that of the two-chain case.

From the discussion in Section 3 related to Fig. 4, we can also conclude that when the number of chains \( M \) increases, \( k_c \) increases and tends to a finite value. As a result, the static friction force (depinning force) \( F_s \) decreases (see in Fig. 5), which means that it is easier to initiate the large model sliding than small model.

5. Conclusion

In this Letter, we have introduced a simple multi-chain Frenkel–Kontorova model and investigated its static properties. We found that the many layer structure presents new dynamic characteristics. The ground state has different configurations in the case of commensurate and incommensurate structures. In the later case, the configuration of each chain is different and can be described by the newly defined hull function \( h(x) \). The transition by the breaking of analyticity also appears in each chain at the same value of \( k_c \), and the critical value at which the transition occurs tends to be finite when the number of chains increases. When the number of chains is fixed, the critical value \( k_c \) increases as the coupling constant \( \gamma \) increases. The hull function \( h(x) \) also shows the transition by breaking of analyticity at the same critical value as that of \( f(x) \). When \( k > k_c \), the behavior of the depinning force can be described by the expression \((k - k_c)^\gamma\). As a model of dry friction, the depinning force is defined as the static friction force. The volume measured by the number of chains \( N \) and hardness measured by the coupling constant between neighboring chains \( \gamma \) play important roles in this field. The static friction becomes small and tends to a finite value when the volume increases. In addition, the slider is easy to begin sliding as the hardness of the sliding body increases.

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