Vol 15 No 7, July 2006
1009-1963/2006/15(07)/1464-07

Chinese Physics

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Nonlinear dynamics in sliding processes: the single-particle case*

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(Received 24 December 2005; revised manuscript received 6 April 2006)

Dynamical behaviours of the motion of particles in a periodic potential under a constant driving velocity by a spring at one end are explored. In the stationary case, the stable equilibrium position of the particle experiences an elasticity instability transition. When the driving velocity is nonzero, depending on the elasticity coefficient and the pulling velocity, the system exhibits complicated and interesting dynamics, such as periodic and chaotic motions. The results obtained here may shed light on studies of dynamical processes in sliding friction.

Keywords: elasticity instability transition , Frenkel–Kontorova model
PACC: 0547

1. Introduction

Tribology, the study of surfaces in moving contact, is a very important field from the viewpoint of technology.[1] The study of sliding friction is one of the oldest problems in physics. In spite of its technological importance and long-term studies, a number of fundamental questions still remain open, especially for an atomistic level understanding.[2−6]

At the atomistic level, the friction dynamics is usually considered as the motion of atoms at the contact level in a periodically corrugated potential. This consideration is closely related to the well-known Frenkel–Kontorova (FK) model.[7] In its simplest form, the FK model consists of a one-dimensional chain of particles coupled by a harmonic nearest-neighbour interaction under the influence of an external spatially periodic potential. The essential physical feature of the model lies in the competition between the following two types of interactions: one of them favours a uniform separation between particles, while the other tends to pin the particles to the bottom of the substrate. This competition, often referred to as the frustration or, more specifically, length scale competition, results in a rich complexity of spatially modulated structures.[8] As experimental and large-scale simulation data at the nanoscale have become available, the more complicated FK-type models have been simulated by using molecular dynamics methods.[9−11] This model has nowadays become very popular in many branches of condensed-matter and nonlinear physics.[12] Especially, from the practical point of view, the driven FK-type models have found intriguing and relevant applications in the field of nanotribology.[13−16]

The FK system has rich and complex dynamics. In some situations, one can ignore interactions between particles and just consider the single-particle dynamics. The motions of one particle in a spatially periodic potential under various forces have been exhaustively investigated in relation to numerous physical problems, such as damped pendulum, phase-locked loops, Josephson junctions,[17] and so on. In spite of long-term efforts, many phenomena still remain unsolved. In this paper, we focus on the sliding dynamics of a particle moving in a periodic potential under the drive of a spring with a constant velocity. We found rich dynamics of this system, which are related

*Project supported in part by the National Natural Science Foundation of China (Grant Nos 70431002 and 10575010), the Foundation for the Author of National Excellent Doctoral Dissertation of China (Grant No 200120), and the Teaching and Research Award Program for Outstanding Young Teachers in Higher Education Institutions, Ministry of Education of China (Grant No 209).

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to different sliding processes. The results we obtained in this paper may be useful in understanding some nonlinear phenomena in tribology.

The paper is organized as follows. In Section 2, we propose the model and discuss the stationary state. The typical elasticity transition is discussed, which manifests well in dynamical cases. The dynamics of a driven particle subject to the periodic substrate potential and a viscous dissipative term is discussed in Section 3. Conclusions are given in Section 4.

2. Sliding process: the stationary case

Let us consider a system that is composed of a particle (say, particle 1) with inertial mass m connected through a spring (with elasticity coefficient K) to another particle (particle 2). The system experiences the corrugated substrate potential $U(q)$ (shown in Fig.1(a)). We concentrate on the dynamical behav-

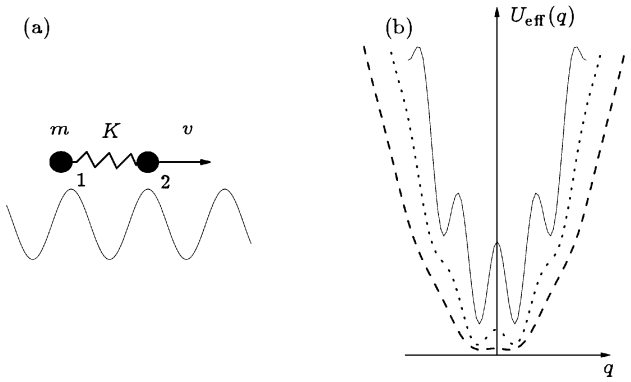


Fig.1. (a) A particle (mass m) connected by a spring (bending force constant K) to another particle and driven by a constant velocity on a corrugated substrate (interaction potential U). (b) The effective potential defined by Eq.(2) at different K. Solid, dotted and dashed lines denote $K = 0.05$, 0.2 and 0.6, respectively.

iour of particle 1, which is governed by the equation of motion

$$m\ddot{q} + m\gamma\dot{q} + U'(q) = K(x - q), \tag{1}$$

where x, q denote the coordinates of the particles. The friction force $-m\gamma\dot{q}$ in Eq.(1) originates from the coupling of the adsorbate to the substrate excitations. That is, $-U'(q)$ is the conservative term, and $-m\gamma\dot{q}$ is the dissipative part of the adsorbate–substrate interaction. Let us define the effective potential:

$$U_{\rm eff}(x, q) = U(q) + \frac{1}{2}K(x - q)^2. \tag{2}$$

Throughout this paper we adopt the case $U(q) = U_0 \cos(2\pi q/a)$ with a being the period of the substrate, and the effective potential is schematically plotted in Fig.1(b) for $x = 0$ and different parameters. It can be found that when K is very large, only the valley located at $q = 0$ exists. When K is decreased, the valley at $q = 0$ is replaced by multiple valleys at $q \neq 0$. In the following discussions we are interested in two cases: (1) x is constant, i.e., x is regarded as an adjustable parameter; (2) x is a time-varying parameter, for example, $x = vt$, which is closely related to various time scales. We first study the equilibrium features of the system. Particularly, we are interested in the equilibrium property of particle 1 as a function of x. In equilibrium state $\dot{q} = 0$ and $\ddot{q} = 0$, thus one has

$$\left(\frac{2\pi U_0}{a}\right) \sin\left(\frac{2\pi q_0}{a}\right) + K(x - q_0) = 0. \tag{3}$$

We assume that the spring is centred at the local maxima of the periodic potential $U(q)$, specifically $x = 0$. Therefore the equilibrium position q_0 satisfies the following equation:

$$\left(\frac{2\pi U_0}{a}\right) \sin\left(\frac{2\pi q_0}{a}\right) = Kq_0. \tag{4}$$

It can be found that q_0 is determined by the cross-point of the straight line $y = q$ and the curve $y = (2\pi U_0/Ka)\sin(2\pi q/a)$, as shown in Fig.2(a). There are two different cases, namely, the case of a 'stiff' spring (A) and the case of a 'soft' spring (B). In case (A), only $q = 0$ is a solution to Eq.(4). While in case (B), three or more solutions exist. More than one solution may exist only when $U_0(2\pi/a)\sin(2\pi q/a) > Kq$, i.e., $K < U_0(2\pi/a)^2$. Since $U''_{\rm eff}(0) = -U_0(2\pi/a)^2 + K < 0$, the $q_0 = 0$ solution is unstable, and the particle will occupy a displaced position (i.e, $q = q_1$ or $-q_1$).

Therefore, a bifurcation from the $q = 0$ solution to two symmetric solutions occurs. This bifurcation is often called the elasticity instability transition (EIT). Further bifurcations to new branches can also be found when K is further decreased, implying the emergence of more metastable states, as shown in Fig.2(b). By introducing the elastic energy $\varepsilon = Ka^2/4\pi^2$, a dimensionless quantity can be introduced:

$$\kappa = U_0/\varepsilon. \tag{5}$$

The EIT occurs when $\kappa > 1$. In the cases of $\kappa < 1$, the existence of multiple metastable states may lead to complicated dynamics when particle 1 is excited in different ways. In the following sections, we are concerned with the simplest case when particle 2 moves with a constant velocity. The responses of the other particle may be quite different, depending on the dragging velocity and other parameters in the system.

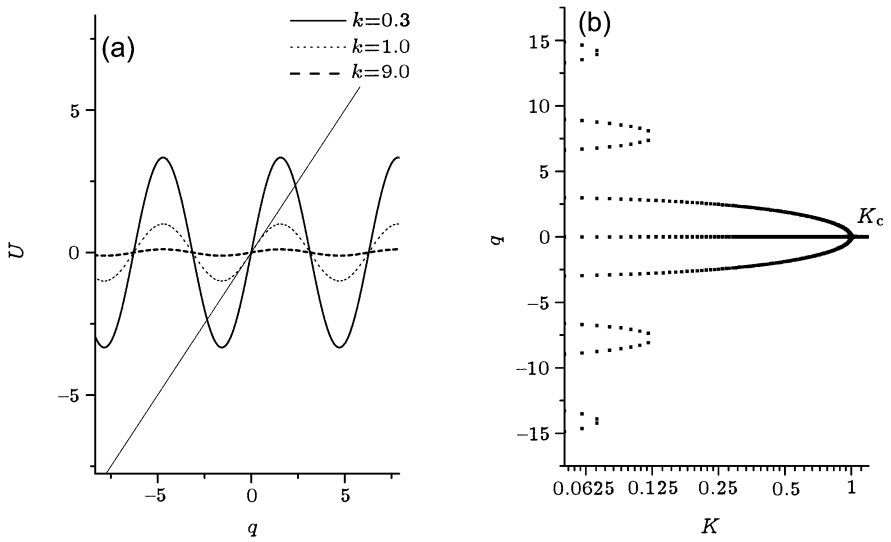


Fig.2. (a) The graphical solution of Eq.(4), which is determined by the crosspoint of the straight line $y = q$ and the curve $y = (2\pi U_0/Ka)\sin(2\pi q/a)$. (b) Stable positions as a function of K.

3. Nonlinear sliding dynamics

Now we consider dynamical behaviours of the motion of particles in the periodic potential under a constant driving velocity by a spring at one end. Suppose now that particle 2 moves with a constant velocity v, i.e., $x = vt$. We first study the limiting case of $v << 1$. As long as $v \neq 0$, particle 1 (below we will replace particle 1 with particle) will slide on the periodic substrate, but it exhibits quite different responses for $\kappa < 1$ or $\kappa > 1$. When $\kappa < 1$, the particle performs a slow oscillatory motion with a frequency $w = Kv$ superimposed on a uniform translation motion vt. This oscillation provides an additional friction on the system. However, due to the stiffness of the spring, the maximum velocity $v_{\max}$ may decrease to 0 as $v \to 0$. This leads to the kinetic frictional force $F_K \to 0$ in the limit of $v \to 0$. On the other hand, when $\kappa > 1$, the particle will always need additional energy to jump from one potential well to another, i.e., the particle exhibits the typical stick-slip motion. Therefore, "fast" motion (sudden sliding motion) of the particle will always be observed, independent of how small the driving velocity v is. This leads to $v_{\max} \neq 0$ as $v \to 0$, and consequently the kinetic frictional force $F_K \neq 0$ in the low-velocity limit. Obviously, the above different dynamics is closely related to the EIT discussed in the equilibrium case.

By introducing the distance between particles 1 and 2, $d = x - q$, Eq.(1) can be transformed to $m\ddot{d} + m\gamma\dot{d} + (2\pi U/a)\sin[2\pi(d - x)/a] = m\gamma\dot{x} - Kd$. For the case $x = vt$, one has

$$\begin{aligned} &m\ddot{d} + m\gamma\dot{d} + (2\pi U/a)\sin[2\pi(d - vt)/a] \\ =&m\gamma v - Kd. \end{aligned} \tag{6}$$

In Eq.(6), the modulation frequency $\omega = 2\pi v/a$ is an important factor for complex dynamics.

In the following numerical simulations, the fourth-order Runge–Kutta algorithm is used to solve the above equation of motion. The time step is small

enough ($\Delta t = 10^{-3}$) to keep the numerical stability, and long-enough integral time interval is adopted to eliminate transient processes. We set $m = 0.01$, $\gamma = 1.0$, $U_0 = 1.0$, $a = 2\pi$. This corresponds to the damping case, and the inertial term plays a significant role in governing the dynamical properties of the sliding process.

In Fig.3(a), we compute the average stretch of the spring $< d >$ against different spring stiffness K. For all cases, $< d >$ increases with increasing driving velocity v and becomes saturated for large v. For large K, the curve is smooth. Some peaks of $< d >$ can be found with increasing v when $K < 1$ ($\kappa > \kappa_c$). These peaks correspond to the resonances between the sliding and the local oscillation. They are regular for small v and become irregular when v is further increased. Another important result is that as $v \to 0$, $d \to 0$ when $K > K_c$ ($\kappa < \kappa_c$), while $< d > \neq 0$ in the case of $K < K_c$. The non-zero stretching of the spring for $K < K_c$ corresponds to the existence of EIT, which is discussed in Section 2. Profiles of the $< d > \sim K$ relation are given in Figs.3(b)–3(d) for different driving velocities. $< d >$ decreases with increasing K and saturates at certain values. Branching behaviour can be found in the weak-coupling regime when v is decreased, indicating the complexity of the sliding process in the weak-coupling limit. To have a better understanding of these complicated branching and resonance behaviours, it is more instructive to study the dynamics of the sliding process. In the damping case, the presence of the inertia term becomes important because it introduces additional time-scale competitions. When the energy provided by the driving cannot be dissipated fast enough by the viscous term $-m\gamma\dot{q}$ in Eq.(1), the inertia term may induce oscillation behaviour. This oscillation will compete with the sliding process and consequently lead to various dynamical motions, such as mode locking (periodic motion), quasi-periodicity, and even chaotic motion.

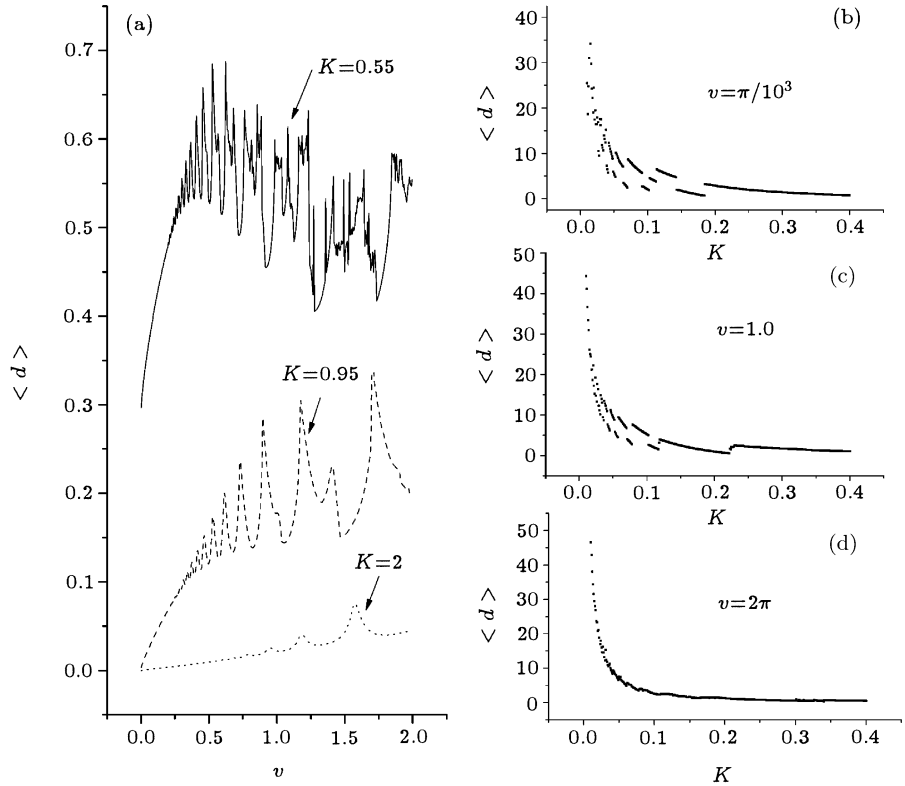


Fig.3. (a) The dependence of $< d >$ on v at different K. (b)–(d) The dependence of $< d >$ on K at different v.

These behaviours also strongly depend on the elasticity coefficient K and the driving velocity. The bifurcation diagram of the velocity of the particle versus K at $v = 2\pi/1000$ is given. Dots in the diagram in Fig.4, represent the instantaneous velocity $v(t) = \dot{q}$ when $q(t)$ passes $2\pi n$ ($n \in Z$). The number of points M for each K denotes a period-M motion. Period-1 motion can be found for strong coupling ($K > 0.19$). Period-2, period-3 and other types of periodic motions can also be observed when K is decreased. Complicated motion is found only in the regime of very weak coupling. We always find periodic motion when the particle is driven with a very slow velocity. When the particle is pulled with a larger v, the motion becomes irregular. This is shown in Fig.5(a), where the bifurcation diagram is given for $v = \pi/3$. One can observe both periodic and chaotic motions. To test whether the motion is chaotic, the reliable quantity is the Lyapunov exponent. When the maximum Lyapunov exponent $\lambda_{\max} > 0$, the motion is chaotic. Figure 5(b) gives the maximum Lyapunov exponent $\lambda_{\max}$ varying with K, which corresponds to Fig.5(a). One can find $\lambda_{\max} > 0$ in many parameter intervals, such as [0.222, 0.24], [0.244, 0.248], [0.254, 0.269]. Many periodic windows can be found between these chaotic regimes.

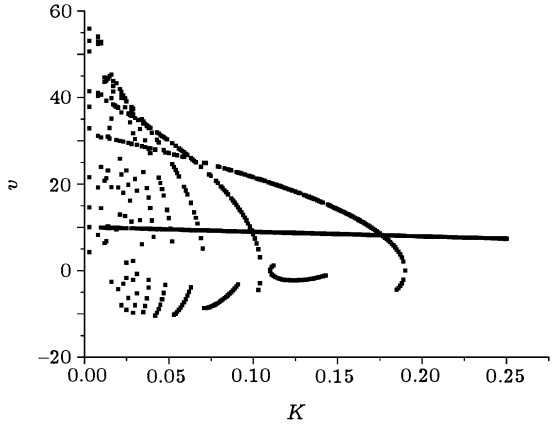


Fig.4. The bifurcation diagram characterized by the velocity of the particle versus K at $v = 0.002\pi$.

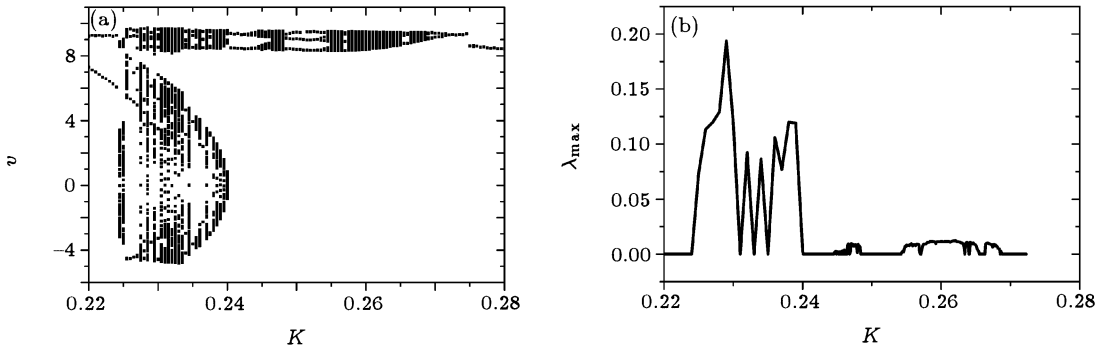


Fig.5. The bifurcation diagram and the corresponding maximum Lyapunov exponent varying with K at $v = \pi/3$.

Because the system always exhibits oscillatory behaviour, no fixed points ($\lambda_{\max} < 0$) can be observed. In Fig.6, we show the bifurcation diagram for three different ranges of K when v is large ($v = 2\pi$). In order to indicate the chaotic motion of the sliding dynamics, the maximum Lyapunov exponent is also plotted. In the weak K regime in Fig.6(a), an intermingled picture of chaotic, periodic, and quasi-periodic motions can be found. Transitions to chaotic motion occur by crisis. When K is very large, as shown in Fig.6(c), the motion is period-1. A transition to chaos with the period-doubling bifurcation can be found when K decreases to a critical value K_c ($K_c \approx 1.0$). In the intermediate coupling regime, as shown in Fig.6(b), both the crisis transition and the period-doubling bifurcation to chaotic motion can be found. This bifurcation is shown in Fig.7, where the velocity of the particle undergoes periods in one period of the substrate potential, with one closed loop representing one period. One can find that when K is varied from 1.2 to 1.15, the number of loop is doubled. When $K = 0.95$ ($\kappa > \kappa_c$), chaotic motion can be found.

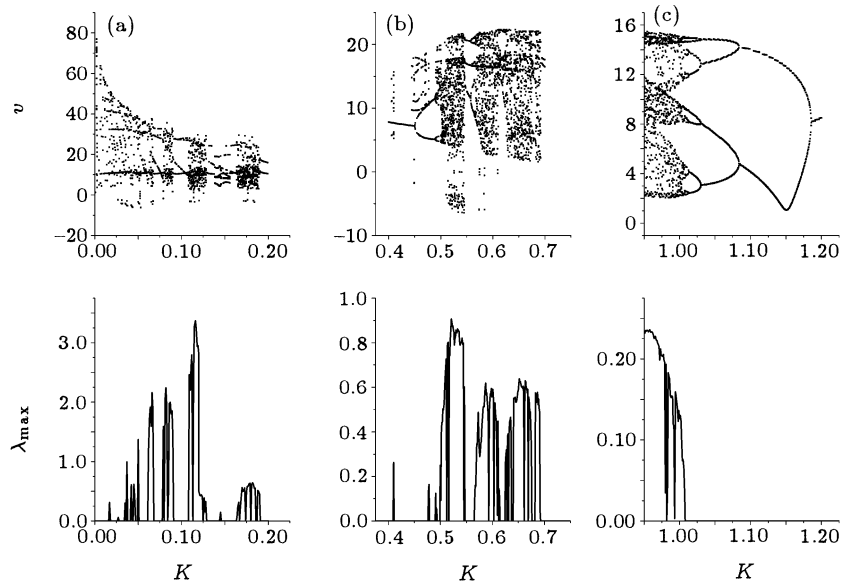


Fig.6. The bifurcation diagrams and the corresponding maximum Lyapunov exponent for three different K at $v = 2\pi$.

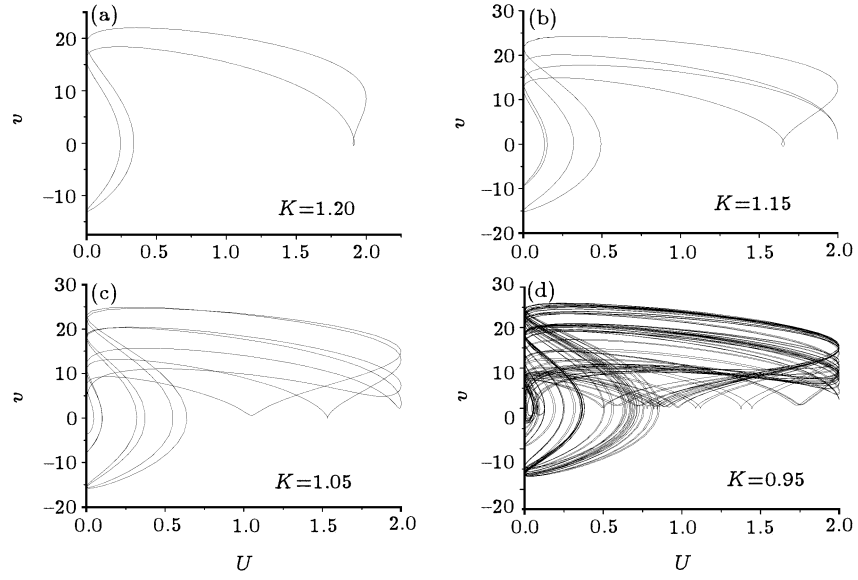


Fig.7. The phase diagram describing the velocity of the particle that undergoes periods in one period of the substrate potential. The four panels show the dynamical behaviours from period-doubling bifurcation at high K to chaos at low K. (a): $K = 1.20$; (b): $K = 1.15$; (c): $K = 1.05$; (d): $K = 0.95$.

4. Concluding remarks

In this paper, we have studied the nonlinear dynamical response of a particle in the periodic substrate potential under a constant driving velocity by a spring at one end. In the equilibrium state, an EIT is shown and discussed. This transition plays an important role in governing the dynamical sliding responses of the particle. We found the transition to chaos via crisis and period-doubling bifurcations. These results reflect the complicated responses of the driven particle in the sliding process. The single particle dynamics discussed in this paper can be regarded as the simplest case of the FK system. When one considers the sliding process of a chain instead of a single particle, the system may exhibit more irregular while quite interesting dynamics. This will be discussed in detail later.

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