A SIMPLE MODEL FOR WEARLESS FRICTION: THE FRENKEL-KONTOROVA-TOMLINSON MODEL

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Abstract. We investigate the static and dynamic properties of a simple model for wearless friction between atomically flat surfaces. The model is a combination of the Frenkel-Kontorova model (a harmonic chain in a spatially periodic potential) and the Tomlinson model (an ensemble of independent oscillators sliding over a corrugated surface). We investigate the ground state, the meta-stable states, the static friction, and the kinetic friction of this model. The static properties strongly depend on the commensurability of the lattice constants of the surfaces. The kinetic properties are dominated by several types of resonance (normal, superharmonic, and parametric resonance).

1. Introduction

When the interfaces of two solid bodies are slided against each other, wear takes place. This is an irreversible process which costs energy and therefore lead to a nonconservative lateral force which is called *friction* [1]. But wear is not essential or even necessary for friction.

In 1929 Tomlinson [2] introduced a mechanism for wearless friction. It also explains why, contrary to viscous friction, dry friction does not vanish when the sliding velocity goes to zero. The idea is that a molecule at one surface can be "plucked" by the other surface, like a guitar string [3]. More precisely: The molecule is pinned at the other surface due to some inhomogeneity, e.g., another molecule. It suddenly depins when the surface is moved further. After the depinning the molecule vibrates. This vibration is damped because the vibrating molecule excites electronic or elastic waves into the bulks of the sliding bodies. This is the dissipation mechanism which leads to friction even in the limit of quasistatic sliding. This friction mechanism is wearless because the plucking of the molecule does not change its equilibrium position. Wearless friction may occur in nanotribology [4, 5].

In this contribution we investigate friction in a model which extends the Tomlinson model by introducing a next-neighbor interaction between the molecules. We call it the Frenkel-Kontorova-Tomlinson (FKT) model because it is a combination of the Tomlinson model and the Frenkel-Kontorova model which is well-known in the field of commensurate-incommensurate transition [6] and charge-density waves [7].

In the next section we introduce the FKT model. We also define static and kinetic friction. In Secs. 3 and 4 we discuss the static and dynamic properties. The results are summaries in the last section.

Figure 1. The Frenkel-Kontorova-Tomlinson model driven by a force F. The position of the upper body and its mass are denoted by x_B and M, respectively. The position of the particle j relative to the support point of the leaf spring is denoted by ξ_j. The distance between subsequent support points is $c = 2\pi l$. The particle mass is $m \equiv 1$ and $\kappa_1 \equiv 1$ and $\kappa_2 \equiv \kappa$ are the stiffnesses of the coil and leaf spring, respectively. The strength of potential describing the lower surface is denoted by b. All parameters and variables are given in dimensionless units.

2. The Frenkel-Kontorova-Tomlinson Model

Figure 1 gives a sketch of the FKT model. Two atomically flat bodies are sliding against each other. One body (the lower one in Fig. 1) is assumed to be rigid whereas the surface atoms of the otherwise also rigid upper body can move freely but only in the sliding direction. The interaction of a surface atom with its nearest neighbors and with the rigid upper body is assumed to be linear which strictly speaking is true only for small displacements out of equilibrium. The interaction with the lower body is described by a periodic potential. We have restricted ourselves to one dimension. The equations of motion read

$$\begin{aligned} \ddot{x}_B + \ddot{\xi}_j + \beta\dot{\xi}_j + \gamma(\dot{x}_B + \dot{\xi}_j) &= \xi_{j+1} - (2+\kappa)\xi_j + \xi_{j-1} \\ &\quad + b\sin(x_B + cj + \xi_j) \qquad (1) \\ M\ddot{x}_B &= F + \kappa\sum_{j=1}^{n}\xi_j. \qquad (2) \end{aligned}$$

For the definition of the variables and parameters see the caption of Fig. 1. The dissipation due to excitation of bulk waves is phenomenologically described by the two damping terms.

We have chosen periodic boundaries

$$\xi_{j+n} = \xi_j \tag{3}$$

which implies that the ratio of the lattice constants

$$l = \frac{c}{2\pi} \tag{4}$$

has to be rational, i.e., $l = p/q$, where p and q are coprime and q is a divisor of n. In order to approximate an irrational ratio a sequence of rational ratios approaching the irrational one has to be investigated. We do this only for the golden mean $(\sqrt{5}-1)/2$ which can be approached by taking for p and q subsequent members of the Fibonacci series, i.e., $\frac{p}{q} = \frac{1}{1}, \frac{1}{2}, \frac{2}{3}, \frac{3}{5}, \frac{5}{8}, \frac{8}{13}, \ldots$

In the following we will investigate only cases where the upper body is in a non-accelerating state, i.e., $\ddot{x}_B = 0$. In the first case the upper body is at rest, i.e., $\dot{x}_B = 0$. We are then investigating the ground state, the meta-stable states, and the static friction. These are static properties of the model. In the other case the upper body slides with finite velocity $\dot{x}_B = v$ and we are interested in the dynamic response of the system. Here we will only discuss the kinetic friction.

2.1. DEFINITIONS OF FRICTION

Before investigating the properties of the FKT model we have to give precise definitions of friction. From (2) follows that the force

$$F(t) = -\kappa \sum_{j=1}^{n} \xi_j(t) \tag{5}$$

has to be applied to the upper body in order to keep it in a non-accelerating state. It should be remarked that this force is simply a lateral force and not a friction force. In order to define friction in models like the FKT model appropriately we have to distinguish between the static friction and the kinetic friction.

2.1.1. *Definition of Static Friction*

In a stationary state where the upper body is not moving and where the atoms are not vibrating the lateral force (5) is in general a non-zero constant which depends on the configuration of the surface atoms and the position of the upper block. To get a definition of the static friction we change our point of view by taking the external force F as the control parameter and not the position of the upper body. We then ask the question, what happens if F is changed quasistatically? The position of the upper body and the positions of the surface atoms will follow F adiabatically until a saddle-node bifurcation is reached where a stable state annihilates with an unstable one. In general the configuration of the surface atoms depins and the system starts to slide. The value of F at the saddle-node bifurcation defines a depinning force which we interpret as the static friction.

In general the depinning force is not the same for all configurations of the surface atoms. Here we see from a very general point of view, why in tribological systems the static friction is not unique but depends on the *history* of the system. Nevertheless we can give a unique definition of the static friction which is independent of the history: *The static friction F_S is the smallest force F for which no stationary state of (1) and (2) exists.* In other words, F_S is the force where the last stationary state disappears. This definition has to be taken with care because it only means that the actual static friction is less than or equal F_S.

2.1.2. *Definition of Kinetic Friction*

If the upper body slides with constant velocity $\dot{x}_B = v$ relative to the lower one the lateral force F defined by (5) will be in general time-dependent. In order to define the kinetic friction F_K we have to take the time average of it

$$F_K(v) = \lim_{T\to\infty} \frac{1}{T}\int_0^T F(t)\,dt = -\lim_{T\to\infty} \frac{\kappa}{T}\int_0^T \sum_{j=1}^{n} \xi_j(t)\,dt. \qquad (6)$$

This definition is equivalent to

$$F_K(v) = \gamma v n + \lim_{T\to\infty} \frac{\beta+\gamma}{vT}\int_0^T \sum_{j=1}^{n} \dot{\xi}_j^2\,dt, \qquad (7)$$

because the work which is put in into the system has to be dissipated totally.

3. Static Properties

In this section we investigate the stationary states and their stability. The stationary states are the solutions of

$$\begin{aligned} 0 &= \xi_{j+1} - (2+\kappa)\xi_j + \xi_{j-1} + b\sin(x_B + cj + \xi_j) & (8)\\ 0 &= \kappa\sum_{j=1}^{n}\xi_j + F. & (9) \end{aligned}$$

These are $n+1$ equations for the n unknown ξ_j's and either the unknown x_B or F. The control parameter is F or x_B, respectively. The stationary states does not depend on which case we have chosen. But the stability and therefore the physical relevance strongly depends on whether F or x_B is the control parameter.

3.1. F AS CONTROL PARAMETER

In order to discuss the static friction F has to be taken as the control parameter. As already mentioned in Sec. 2.1.1, the static friction is the force F at which the last stationary state disappears. This last state has to be that which is most strongly pinned. Intuitively it is clear that this is the ground state of the undriven (i.e., $F = 0$) system.

Figure 2. The hull function g_S for the golden mean $l = (\sqrt{5} - 1)/2 \approx 144/233$ and $\kappa = 1$. Solid (dotted) line corresponds to $b = 2.5$ (3) which is below (above) the point of breaking of analyticity of the hull function.

3.1.1. *The Ground State for $F = 0$*

For $b = 0$ the ground state is simply $\xi_j = 0$. For $b \neq 0$ the ground state is as close as possible to this state in order to minimize the energy stored in the springs. We find that the ground state is uniquely determined by the fact that each particle lies in the potential well which is underneath the support of its leaf spring (see Fig. 1). Similarly to the Frenkel-Kontorova model [8], the ground state is given by a *hull function* g_S:

$$\xi_j = g_S(x_B + cj), \quad \text{with} \quad g_S(x + 2\pi) = g_S(x) = -g_S(-x). \tag{10}$$

The properties of g_S are reflecting the symmetries of the system.

In the commensurate case x_B is restricted to the finite set

$$x_B = \left(\frac{1}{2} + k\right)\frac{\pi}{q}, \quad k \text{ integer}, \tag{11}$$

which is determined by symmetry arguments. It lead to a degeneracy of the ground state where x_B can be interpreted as a phase.

In the incommensurate case x_B can be any arbitrary real value. Figure 2 shows numerical approximations of the hull function for an incommensurate ratio l. We clearly see a manifestation of Aubry's breaking of analyticity: For $b = 2.5$ the curve is smooth whereas for $b = 3$ the curve has an infinite number of steps densely distributed. We denote the point of breaking of analyticity as b_c^S. Because x_B can be arbitrary, a Goldstone mode exists below b_c^S. Therefore, the ground state is not pinned and can be shifted by an infinitesimally small force.

3.1.2. *The Meta-stable States for $F = 0$*

For $b = 0$ the ground state is the only stationary state. If b exceeds some critical value $b_c^K > 0$ additional stationary states appear which are stable for x_B fixed but unstable for x_B free. If b exceeds a further threshold $b_c^m \geq b_c^K$ the first of these stationary states becomes stabilized, i.e., the first meta-stable state appears. It is a pair of a phase kink and anti-kink which separate two equally sized domains. The domain states are slightly deformed ground states. The domains are characterized by the different values of the ground state phase (11). The difference between both phases is π/q. The block position x_B (i.e., the real x_B not the "virtual" ones of the domains) is the average over the domain phases. Thus x_B is an integer multiple of π/q. For the commensurate ratio $l = 1$ we are able to calculate the thresholds analytically:

$$b_c^K = \kappa, \quad b_c^m = \frac{\pi}{2}\kappa, \quad \text{for} \quad l = 1. \tag{12}$$

Numerically we always found $b_c^m > b_c^K$ for commensurate ratios l. For the incommensurate case, b_c^m, b_c^K, and b_c^S appear to be identical.

Figure 3. The static friction F_S as a function of b for $\kappa = 1$. Thin lines denote curves for $l = 1/2, 2/3, 3/5, 5/8, \ldots$ whereas the thick line denotes $l = (\sqrt{5} - 1)$.

3.1.3. *The Static Friction*

As already mentioned above, if F is gradually turned on, the stable stationary state which disappears at last will be that which develops adiabatically from the ground state. We have not found in numerical checks with several meta-stable states and different values of q any example demonstrating the opposite. But it is hard to prove this statement rigorously. We can prove it only for $l = 1$ where the static friction F_S is equal to the overall upper limit F_S^{max}. For the proof we replace (5) by

$$F = -b \sum_{j=1}^{n} \sin(x_B + cj + \xi_j), \tag{13}$$

which is obtained by taking the sum over (8). We immediately see that the overall upper limit is

$$F_S^{max} = bn. \tag{14}$$

Furthermore, for $l = 1$ all ξ_j's of the state which develops adiabatically from the ground state are identically. Thus

$$F_S = F_S^{max} = bn, \quad \text{for} \quad l = 1. \tag{15}$$

Figure 4. The threshold b_c as a function of κ. Thin lines denote b_c^K for $l = 1, 1/2, 2/3, 3/5, \ldots$ whereas the thick line denotes $b_c^S = b_c^K = b_c^m$ for $l = (\sqrt{5}-1)/2$.

From our numerical calculation we find that in the commensurate case F_S is a strictly monotonic function of b with $F_S(0) = 0$. Figure 3 shows F_S as a function of b for a sequence of l approaching the golden mean $(\sqrt{5}-1)/2$. In the asymptotic limit we get F_S for the golden mean which has a singularity at $b = b_c^S$. For $b < b_c^S$ the static friction is zero because of the existence of a Goldstone mode. For $b > b_c^S$ it is a strictly monotonic function of b which near b_c^S scales like

$$F_S(b) \sim (b - b_c^S)^\nu, \quad \text{with} \quad \nu \approx 2. \tag{16}$$

This is similar to the Frenkel-Kontorova model except that the scaling exponent there is roughly three [9]. Figure 4 shows $b_c \equiv b_c^S = b_c^K = b_c^m$ as a function of κ for the golden mean. For $\kappa \to 0$ it approaches the well-known value of the point of breaking of analyticity of the Frenkel-Kontorova model [9], i.e., $b_c(0) \approx 0.97$. Near zero b_c scales like

$$b_c(\kappa) - b_c(0) \sim \kappa^\mu, \quad \text{with} \quad \mu \approx \frac{1}{2}. \tag{17}$$

We now reinterpret b_c^S as the threshold for the occurrence of static friction. In the commensurate case b_c^S is always zero which means that there is always static friction.

3.2. X_B AS CONTROL PARAMETER

In the case of x_B as control parameter we have to solve only the n equations (8) instead of the $n+1$ equations (8,9). If there is only one unique solution for any value of x_B the kinetic friction in the quasistatic limit $v \to 0$ will be zero because the state adiabatically follows x_B. It therefore does not dissipate energy. The lateral force F is then a periodic function of x_B which is on average zero. What happens with $F(x_B)$ if we increase b? It will develop a loop and above some critical value of b it will be no longer a unique function of b because at least two saddle-node bifurcations emerge and make the system at least bistable. If x_B is swept quasistatically over such a saddle-node bifurcation the system will suddenly jump into another stable state. This is Tomlinson's basic friction mechanism. In our numerical study we always find that the threshold of occurrence of finite kinetic friction in the quasistatic limit is identical with b_c^K. Figure 4 shows b_c^K as function of κ for a sequence of commensurate ratios l approaching the golden mean.

4. Dynamic Properties

In this section we discuss the mechanisms leading to kinetic friction at finite sliding velocities, i.e., $x_B = vt$. As already mentioned in the introduction the basic mechanism is the excitation of bulk waves due to vibrations of the surface atoms. The rate of dissipation into these channels are given by the damping constants β and γ. But how strongly are these channels fed and how is the lateral motion turned into atomic vibrations?

For $b = 0$ the atoms do not vibrate, i.e., $\xi_j = 0$. Only the motion of the atoms relative to the lower body leads to dissipation which yields $F_K = \gamma vn$. This is the first term of (7). It is an unavoidable background. In the following we always drop this background. This is equivalent to eliminating the dissipation channel into the lower body and replacing the dissipation rate into the upper body by the sum of both rates. This means formally that we set in the equation of motion (1) $\gamma = 0$.

4.1. WEAK INTERACTIONS

For small but non-zero values of b the vibrations will also be small. Thus in leading order in b we can neglect ξ_j in the nonlinear term. This leads to a linear equation of motion which can be immediately solved. The solution is

$$\xi_j = \frac{b\cos(vt + cj + \phi)}{\sqrt{[\omega^2(c) - v^2]^2 + \beta^2 v^2}}, \tag{18}$$

where $\omega(k)$ is the phonon dispersion relation

$$\omega(k) = \sqrt{\kappa + 4\sin^2\frac{k}{2}}. \tag{19}$$

Using (7) we get

$$\frac{F_K(v)}{n} = \frac{\beta v b^2/2}{[\omega^2(c) - v^2]^2 + \beta^2 v^2}. \tag{20}$$

Thus the kinetic friction has a *resonance peak* at the frequency of the phonon with wave number $k = c$.

In the next step we linearize the nonlinear term in the equation of motion (1). In addition to the term $b\sin(vt+cj)$ we get $b\cos(vt+cj)\cdot\xi_j$ which is responsible for *superharmonic resonances* and *parametric resonances*.

4.1.1. *Superharmonic Resonance*

In superharmonic resonances higher harmonics also cause resonance because of the coupling between different harmonics due to the term $b\cos(vt+$

$cj) \cdot \xi_j$. The superharmonic resonance velocities are

$$v_m^S = \frac{\omega(mc)}{m}, \quad m \text{ integer}. \tag{21}$$

The normal resonance is therefore only a special case ($m = 1$) of this more general kind of resonance. Superharmonic resonance is simply the effect that an oscillator also shows resonance if it is kicked only at every m-th oscillation. The strength of the resonance is of course weaker than in the normal case. In the language of solid-state physics superharmonic resonance is the decay of m waves with wave number c and frequency v into one phonon with wave number k and a frequency $\omega(k)$. The conservation of momentum and energy immediately leads to (21).

4.1.2. *Parametric Resonance*
Another effect of the term $b\cos(vt+cj)\cdot\xi_j$ is parametric resonance. It always occur when the eigenfrequency of an oscillator is modulated. The prototype of parametric resonance is a mathematical pendulum with a vertically oscillating support. Parametric resonance is a threshold phenomenon. If the modulation strength is below the threshold the pendulum will not swing. Above the threshold a parametrically driven oscillator starts to oscillate. At the beginning, the oscillation amplitude increases exponentially. Contrary to the other types of resonances the saturation of the amplitude is not given by the damping rate but by the nonlinear terms of the equation of motion.

The threshold as a function of the driving frequency has characteristic minima. These minima occur for frequencies where the eigenfrequency of the oscillator is an integer multiple of half the driving frequency. This is the so-called parametric resonance condition. The integer multiple defines the order of parametric resonance. The first order parametric resonance has the lowest threshold which is proportional to the damping constant.

What is the parametric resonance condition in systems, like the FKT model, which are driven by a wave? The answer can be found by using again the intuitive picture from solid state physics: In the m-th order parametric resonance m waves with wave number c and frequency v decay into two waves with wave number k_1 and k_2 and frequencies $\omega(k_1)$ and $\omega(k_2)$ where the momentum and energy is conserved. This leads to

$$v_m^P(k) = \frac{\omega(mc/2 + k) + \omega(mc/2 - k)}{m} \tag{22}$$

where k is an arbitrary number which is restricted to integer multiples of $2\pi/n$ in the case of a finite system. The minimum and maximum of $v_m^P(k)$ define an interval of velocities for which phonons will be excited parametrically if b exceeds some threshold. In this interval we expect a larger kinetic friction. But we are not able to calculate F_K analytically because the nonlinearities become essential.

Figure 5. The kinetic friction F_K as a function of the sliding velocity v for $b = \kappa = 1$, $\beta = 0.1$, $\gamma = 0$, and $N = 233$. (a) The incommensurate case $l = (\sqrt{5} - 1)/2) \approx 144/233$. (b) The most commensurate case $l = 1$. In each simulation v was successively changed by steps of size 0.05 from zero to some finite value (solid lines, squares) and back to zero (dashed lines, triangles). After each change 10^3 time units has been waited because of possible transients. After that the force was calculated in accordance to (6) with $T = 100\pi/v$. This calculation was repeated ten times. The mean value and the standard deviation (error bar) are shown. Arrows denote normal, superharmonic, and parametric resonances in accordance to (21) and (22).

4.1.3. *Numerical results*

Figure 5 shows the results of numerical calculations of $F_K(v)$. We can clearly identify normal resonance, superharmonic resonance as well as parametric resonance. The peak of normal resonance is not as high as one would expect from (20). The reason is that the energy is not only dissipated directly in the bulk but also into other phonon modes due to the nonlinearity. This leads to an effectively higher damping constant.

Whether the lattice constant ratio l is commensurate or incommensurate does not play an important role. Only the positions of the resonance peaks and the first-order parametric resonance window are shifted in accordance with (21) and (22). But the values of F_K at these resonances are comparable. Considerable differences are recognizable only for sliding velocities below v_1. They are mainly caused by the fact that for the parameters of Fig. 5(b) b is just at the threshold b_c^K where the kinetic friction starts to becomes non-zero (see also Fig. 4).

In the parametric resonance window one can clearly see that F_K can have different values. Therefore the kinetic friction is not uniquely defined. It also depends on the history of the system.

For velocities larger than the maximum of v_1^P the kinetic friction is almost zero because the surface atoms of the upper body only perform tiny oscillation around their equilibrium position. Thus the surface is solid. We call this state the *solid-sliding state*.

Figure 6. Same as in Fig. 5 but for $b = 4$.

4.2. STRONG INTERACTION

In the case of strong interaction the resonance peaks are smeared out. A typical example is shown in Fig. 6. Only the normal resonance peak and the left and right wing of the first-order parametric resonance window survive. The motion of the system is strongly chaotic even in the surviving resonance peaks. Right of the first-order parametric resonance window a broad shoulder with some small peaks has appeared. Here the system is strongly bistable between the chaotic state and the solid-sliding state.

The overall picture is that the kinetic friction first decreases, then increases, reaching a maximum near the normal resonance, before it decreases again.

5. Conclusion

In this contribution we have discussed some static and dynamic properties of a simple model for wearless friction, the Frenkel-Kontorova-Tomlinson model.

The static properties strongly depend on whether the ratio of the surface lattice constants is commensurate or incommensurate. This influences the occurrence of meta-stable states in the undriven case (i.e., no external force), of static friction F_S, and of kinetic friction F_K in the quasistatic limit (i.e., sliding velocity $v \to 0$). It can be expressed in terms of thresholds for the strength b of the interaction between the sliding surfaces. That is, if b is less than b_c^m, b_c^S, and b_c^K meta-stable states do not exist, $F_S = 0$, and $F_K(v \to 0) = 0$, respectively. For the commensurate and incommensurate case we found $b_c^S = 0 < b_c^K < b_c^m$ and $0 < b_c^S = b_c^K = b_c^m$, respectively. Thus zero kinetic friction in the commensurate case does not imply zero static friction. This is the case only in the incommensurate case.

The kinetic friction for finite velocities is strongly determined by several types of resonances. The normal and superharmonic resonances lead to well defined peaks which smoothly emerge with increasing b. On the other hand, the parametric resonance is a threshold phenomenon. To excite vibrations b has to exceed some threshold which is proportional to the dissipation rate $\beta + \gamma$. Above the threshold the kinetic friction abruptly increases to values which are often as large as the peak of the normal resonance. This occurs over a finite interval in the sliding velocity v.

The static friction as well as the kinetic friction are not uniquely defined. They depend on the history of the system. This dependence is usually attributed to wear. But the FKT model shows that this need not be the case. The reasons for that are the existence of many meta-stable stationary states and the multistability of dynamical attractors. These are generic properties of many nonlinear systems. Thes even hold for a single Tomlinson oscillator [10, 11].

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