Dry friction in the Frenkel-Kontorova-Tomlinson model: Static properties

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We investigate wearless friction in a simple mechanical model called the Frenkel-Kontorova-Tomlinson model. It combines the Frenkel-Kontorova model (i.e., a harmonic chain in a spatially periodic potential) with the Tomlinson model (i.e., independent oscillators connected to a sliding surface in a fixed potential describing the other surface). We investigate static properties like the ground state, the metastable states, and static friction, as well as the kinetic friction in the limit of quasistatic sliding. As in the Frenkel-Kontorova model the behavior strongly depends on whether the ratio of lattice constants is commensurate or incommensurate. In the incommensurate case, Aubry's transition by breaking of analyticity also appears in the Frenkel-Kontorova-Tomlinson model. The behavior depends strongly on the strength of the interaction between the sliding surfaces. For increasing interaction, we find three thresholds which denote the appearance of static friction, of kinetic friction in the quasistatic limit, and of metastable states in that order. These are identical only in the incommensurate case. In the commensurate case, static friction can be nonzero even though the kinetic friction vanishes for sliding velocity going to zero.

I. INTRODUCTION

Dry friction is a phenomenon of everyday life. Since Coulomb's work its basic phenomenological laws are well known:[1] (i) The friction force is independent of the area of the sliding surface. (ii) It is proportional to the load. (iii) The kinetic friction, i.e., the force to keep a body sliding at a constant velocity, does not depend on the velocity and it is less than or equal to the static friction, i.e., the force to start sliding. On a macroscopic level, these laws are well understood in terms of the Bowden-Tabor adhesion model,[1,2] which is a macroscopic model based on the elastic and plastic properties of the sliding bodies.

In spite of the simplicity of Coulomb's laws, the sliding of two solid bodies is a very complex phenomenon that operates mostly far away from thermal equilibrium. It involves processes on various spatial and temporal scales, from microscopic to macroscopic (for an overview of the state of the art see Ref. 2). Also, deviations from Coulomb laws have been found, which depend on the material of the sliding bodies, the surface properties, the sliding history, and the mechanical environment. Up to now no generally accepted theory exists which is able (i) to explain these deviations and (ii) to calculate friction forces from the bulk and surface properties of the sliding bodies. However, in recent years modern experimental technologies have made it possible to study wearless friction between clean and atomically flat surfaces.[2] There is some hope that theoretical models will lead to an understanding of such less complex systems.

The first attempt to explain Coulomb's laws on the atomic level was given by Tomlinson[3] in his pioneering work in 1929. He considered the surface atoms as single independent oscillators that are "plucked" by the atoms of the other surface like a guitar string. Even quasistatic sliding (i.e., sliding at an infinitesimally small velocity) will lead to plucking of atoms if the stiffness of the interaction between a surface atom and the bulk is smaller than the stiffness of the interaction between this atom and an atom from the other surface at the moment of closest contact.[4,5] During plucking the atom is assumed to jump abruptly from one equilibrium position to another. Such jumps lead to vibrations of the jumping atom. The kinetic energy of the vibrating atom is assumed to dissipate totally into the bulk of the sliding bodies due to excitation of some kind of waves. Thus finite friction is possible even in the limit of zero sliding velocity, contrary to viscous friction, which vanishes in the quasistatic limit. The assumptions that the jumps occur instantaneously and that the atoms are uncoupled, i.e., a vibrating atom does not excite vibrations of other atoms, lead to Coulomb's third law.[3,5]

The easiest model for taking into account the coupling between atoms is the Frenkel-Kontorova (FK) model,[6] which is a model of an adsorbed monolayer on an atomically flat surface. It is a one-dimensional model with a chain of adsorbate atoms coupled linearly by nearest-neighbor interactions. The chain interacts with a spatially periodic potential. The FK model has also been used as a simple friction model.[7,4,5] The static properties of this model strongly depend on the ratio of the lattice constants of the adsorbate layer and the substrate surface. Aubry has shown[8] that, in the case of an irrational ratio, the ground state can be shifted by an infinitesimally small force as long as the strength of the periodic potential is below a critical value (the point of analyticity breaking). Thus the static friction is zero. This is true only in the thermodynamic limit, i.e., in the case of an infinite number of adsorbate atoms.

There is some ambiguity in the literature concerning the meaning of the term *frictionless*. In the context of the FK model frictionless means zero static friction. Another meaning of frictionless found in the literature is a vanishing kinetic friction in the limit of infinitesimally slow sliding.[4] Recently this notion has been called *superlubricity*,[9,10] which is a misleading term because it does *not* imply that a *finite* sliding velocity exists below which the kinetic friction is zero. It should be emphasized that the two definitions of frictionless are *not* equivalent. Of course, zero static friction implies zero kinetic friction if we believe in Coulomb's third

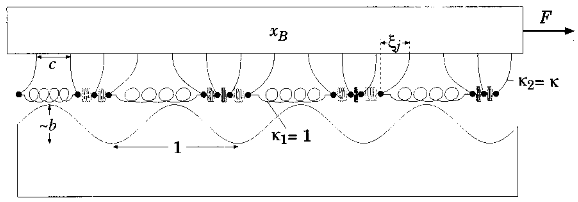

FIG. 1. The Frenkel-Kontorova-Tomlinson (FKT) model where x_B is the position of the upper sliding body, F is the applied force, c is the lattice constant of the surface of the upper sliding body, κ_1 and κ_2 are the stiffness constants of the coil and the leaf springs, respectively, ξ_j is the position of particle j relative to the support of its leaf spring, and b is the strength of the interaction with the surface of the fixed rigid lower body. Its lattice constant defines the length unit. The stiffness of the coil springs defines the unit of the strength of interaction.

law. But a vanishing kinetic friction does not imply a vanishing static friction. This can be easily seen in the Tomlinson model: When the interaction of the oscillator with the sliding surface is weak, it will not be plucked. Thus it can be moved adiabatically without dissipation and the kinetic friction is zero. Nevertheless, the surface *pins* the oscillator. Therefore a finite force is necessary to depin it, which means that the static friction is not zero. It is equal to the amplitude of the oscillating sliding force in the case of adiabatic sliding.

The main disadvantage of the FK model is that the atoms are not coupled to the sliding body. One simple way to overcome this disadvantage is to couple each atom harmonically to a rigid body (see Fig. 1). The resulting model we call the Frenkel-Kontorova-Tomlinson (FKT) model because it is a combination of the FK model and the Tomlinson model.

The FKT model is similar to the Burridge-Knopoff (BK) model,[11] which was proposed as a model of an earthquake fault. The main difference is that in the BK model the interaction with the lower body is replaced by a phenomenological dry friction law. Usually a velocity-weakening law is chosen.[12] For small sliding velocities, this model exhibits avalanches (i.e., earthquakes). For that reason the BK model has become a popular model for the investigation of self-organized criticality.[12,13] Also, solitonlike behavior has been found.[14]

This paper is the first part of a series of papers investigating the FKT model. This part considers only the static properties. The forthcoming parts will be devoted to kinetic friction and stick-slip motion, respectively. This first part is organized as follows: Section II introduces the FKT model. Section III investigates the FKT model in the case of zero driving force. In Sec. IV we calculate the static friction. The kinetic friction in the quasistatic limit is considered in Sec. V. We conclude with Sec. VI.

II. MODEL

The Frenkel-Kontorova-Tomlinson (FKT) model is a one-dimensional lattice model for the atomic monolayer of the surface of a soft body (upper body in Fig. 1) which slides on a hard body (lower body in Fig. 1). The monolayer is described by a chain of N particles with harmonic nearest-neighbor interactions (coil springs). The interaction of each particle with the otherwise rigid upper body is also harmonic (leaf springs). The equilibrium positions of the particles due to this interaction define a regular lattice where the lattice constant is assumed to be the bulk lattice constant of the upper body. The interaction of the particles with the lower body is described by a spatially periodic external potential, which defines a hard surface. The lower body is assumed to be fixed whereas the upper body is movable. The model assumes motions only *parallel* to the sliding surface.

The potential energy of the FKT model is

$$V(\xi_1,\ldots,\xi_N,x_B)=\frac{1}{2}\sum_{j=1}^{N}(\xi_j-\xi_{j-1})^2+\frac{\kappa}{2}\sum_{j=1}^{N}\xi_j^2+\frac{b}{2\pi}\sum_{j=1}^{N}\cos 2\pi(x_B+cj+\xi_j)-Fx_B. \tag{1}$$

Here c is the lattice constant of the upper body, x_B is the position of the upper body relative to the lower surface, ξ_j is the position of particle j relative to the support x_B+cj of its leaf spring, κ is the stiffness of the leaf springs, b is the strength of the external potential that models the interaction with the lower body, and F is the force applied to the upper body. All variables and parameters are measured in dimensionless units. They are based on the following independent basic units: The length unit is the surface lattice constant of the lower body, and the unit of the interaction strength is the stiffness of the nearest-neighbor coupling. All other units can be expressed in terms of these basic units.

We choose periodic boundaries

$$\xi_{j+N}=\xi_j. \tag{2}$$

This implies a rational upper lattice constant c because cN has to be an integer

$$c=\frac{P}{Q}, \tag{3}$$

where P and Q are coprime, and Q is a divisor of N.

For $F\neq 0$ the potential energy V is not bounded from below. Thus no ground state exists and all local minima correspond to metastable states. Therefore, the system is always in a nonequilibrium state. At finite temperature, the system can escape from a metastable state to another metastable state with lower energy. Thus the system creeps due to thermal activation.[15] In this paper we restrict ourselves to zero temperature.

The FKT model is invariant against the following transformations.

(i) *Translations* by an integer multiple of the lattice constant of the lower body generated by

$$x_B\rightarrow x_B+1. \tag{4a}$$

(ii) *Cyclic permutations* of the deformations ξ_j generated by

$$x_B \to x_B + c, \quad \xi_j \to \xi_{j+1}. \tag{4b}$$

(iii) *Reflection* of the upper body at $x=0$:

$$x_B \to -x_B, \quad \xi_j \to -\xi_{-j}, \quad F \to -F. \tag{4c}$$

(iv) *Rescalings* of the lattice constant, generated by

$$c \to c+1. \tag{4d}$$

(v) *Inversion* of the counting order:

$$c \to -c, \quad \xi_j \to \xi_{-j}. \tag{4e}$$

These transformations leave the energy landscape invariant, except for the fact that (4a) and (4b) shift the potential by a constant value proportional to F. The symmetries (4) hold also for an arbitrary periodic potential, except for the reflection symmetry (4c), which holds only for potentials that are invariant against reflection like the cosine potential in (1). The symmetries permit us to restrict c to the interval $[1/2,1]$.

For $\kappa=0$ the FKT model becomes the FK model. For $\kappa, b \to \infty$ but b/κ finite, or similarly by dropping the nearest-neighbor interaction, the FKT model turns into the Tomlinson model of independent oscillators.

As in the case of the FK model, we expect a strong dependence of the FKT model on whether c is rational or irrational. There are two extreme cases: (i) The most commensurate case, $c=1$, and (ii) the most incommensurate case given by the golden mean $c=(\sqrt{5}-1)/2=0.618\ldots$. In order to treat the latter case we have to investigate a series of FKT models with successively increasing numbers of particles. Since continued fractions are the optimum rational approximations of irrational numbers, we take successive pairs from the Fibonacci series 1,1,2,3,5,8,13, ... in order to approximate the golden mean.

III. FKT MODEL WITHOUT DRIVING

In this section we investigate the FKT model where the external force is absent, i.e., $F=0$. Stationary states are the extrema of (1), which are solutions of

$$0=-\partial_{\xi_j}V=\xi_{j+1}+\xi_{j-1}-(2+\kappa)\xi_j+b\sin 2\pi(x_B+cj+\xi_j), \tag{5a}$$

$$0=-\partial_{x_B}V=\kappa\sum_{j=1}^{N}\xi_j. \tag{5b}$$

It is important to note that x_B is not a free variable, because a state that is stationary with respect to the ξ_j need not be stationary with respect to x_B.

Because of the symmetries (4a), (4b), and (4c) any solution can be generated from a solution with

$$x_B \in \left[0, \frac{1}{2Q}\right]. \tag{6}$$

For $F=0$, the potential energy (1) of the FKT model is bounded from below. Thus a *ground state* exists. It strongly determines the static friction, as we will see below.

A. Ground state

In order to calculate the ground state, we start with the trivial case $b=0$ where the energy surface is a paraboloid in the N-dimensional configuration space defined by $\{\xi_j\}$. Equation (5b) defines a plane in this configuration space on which the solution is situated. The absolute minimum of the parabolic energy surface is at $\xi_j=0$. This solution automatically fulfills (5b). Thus x_B is arbitrary.

In the general case, $b\neq 0$, the external potential adds some corrugation onto the parabolic energy surface, which shifts the absolute minimum a certain amount outside the origin. By changing x_B, this minimum can be moved into the plane defined by (5b). Thus, the ground-state position x_B^G of the upper body is no longer arbitrary. The deformations ξ_j^G of the absolute minimum in any direction cannot exceed half the periodicity of the external potential:

$$|\xi_j^G|\leq \tfrac{1}{2}, \quad j=1,\ldots,N. \tag{7}$$

For small values of b the ξ_j^G's are linear in b. For $b\to\infty$ the particles are situated in the local minima of the external potential. In order to minimize the potential energy in the springs, each particle will presumably sit in that potential well that is directly underneath the support of the leaf spring (see Fig. 1). Thus we conjecture that, for the ground state,

$$\mathrm{Int}(x_B^G+cj+\xi_j^G)=\mathrm{Int}(x_B^G+cj), \quad j=1,\ldots,N \tag{8}$$

holds. The same property holds for the ground state of the FK model,[8] where c corresponds to the winding number. Numerically we have not found any example demonstrating the opposite. Furthermore, we found that any other state violates (8). Thus the ground state is uniquely defined by (8). Note that (7) and (8) are independent conditions. The ground state is either *commensurate* or *incommensurate* depending on whether c is rational or irrational.

Aubry has shown[8] that the ground state of the FK model can be uniquely described by a *hull function*. This concept can also be applied to the FKT model. Thus we write

$$\xi_j^G=g_S(x_B^G+cj). \tag{9}$$

From Eq. (5a), the hull function g_S is a solution of the delay equation

$$0=g_S(x+c)+g_S(x-c)-(2+\kappa)g_S(x) + b\sin 2\pi[x+g_S(x)], \tag{10}$$

where $x=x_B^G+cj$. Assuming that the ground state does not break the symmetries (4) we get

$$g_S(x+1)=g_S(x)=-g_S(-x). \tag{11a}$$

The properties (7) and (8) are equivalent to

$$|g_S(x)|\leq 1/2 \tag{11b}$$

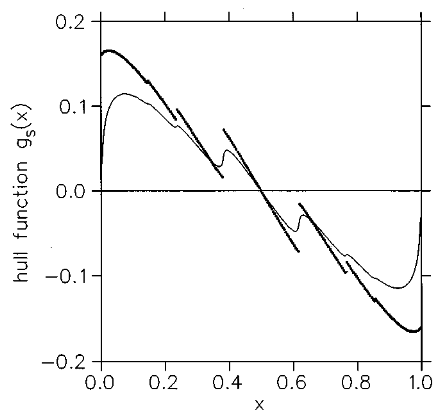

FIG. 2. The hull function $g_S(x)$ for $\kappa=1$ and $c=(\sqrt{5}-1)/2\approx 144/233$. Solid line: $b=0.4$. Dotted line: $b=0.5$.

and

$$|g_S(x)+x \bmod 1-1/2|\leq 1/2, \qquad (11c)$$

respectively.

Which values of x_B fulfill Eq. (5b)? First we consider the commensurate case. Because of the symmetries (4), every x_B with $x_B \bmod(1/2Q)=0$ yields a stationary state. Numerically we find that the ground state is given by

$$x_B^G=\left(\frac{1}{2}+n\right)\frac{1}{Q}, \quad n \ \text{integer}. \qquad (12)$$

In the incommensurate case x_B is arbitrary. We can interpret x_B as a *phase* which is discrete for rational values of c and continuous for irrational ones. Below we will see that this interpretation becomes very important for the construction of elementary defect solutions.

Figure 2 shows the hull functions of numerically calculated ground states for an incommensurate value of c. We clearly see that they fulfill the properties (11). Figure 2 also shows the phenomenon of *breaking of analyticity*, first discovered by Aubry[8] in the FK model. It means that in the incommensurate case the hull function is no longer analytic for b above a certain critical value b_c^S. The nonanalyticity is caused by jumps that appear at certain points. The biggest jump is at $x=0$. It means that a kind of forbidden region has emerged around the maxima of the external potential where no particle is allowed to be. Due to the nearest-neighbor interaction, jumps also appear at $x=cn$, n integer. The size of the jumps decreases with increasing order $|n|$. Since the hull function is a periodic function and c is an irrational number, jumps occur in any neighborhood of any point $x\in[0,1]$.

In the commensurate case only Q jumps occur. In Sec. V we will see that, in any case, whether commensurate or incommensurate, the occurrence of jumps in the hull function corresponds to the occurrence of kinetic friction in the quasistatic limit.

It is possible to show as for the FK model that in the incommensurate case a transition by breaking of analyticity must exist. First we show that for b smaller than some $b_1>0$ the hull function is analytic. This statement is much easier to prove than the similar statement for the FK model

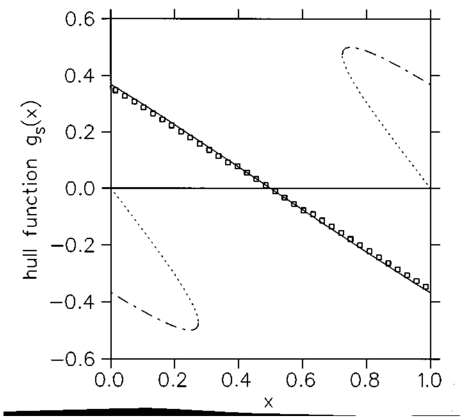

FIG. 3. The hull function $g_S(x)$ in the Tomlinson limit (i.e., $\kappa,b\to\infty$) defined by (15) with $b/\kappa=0.5$. The solid line indicates stable states of a single Tomlinson oscillator with fixed support x. Dashed-dotted and dotted lines indicate metastable states and unstable states, respectively. The squares denote the ground state of the FKT model for $\kappa=10$, $b=5$, and $c=21/34$.

where the Kolmogorov-Arnold-Moser (KAM) theorem is needed because of small denominators. In the FKT model we do not have the small-denominator problem because for $b=0$ the dispersion has a gap. Thus we can apply the implicit function theorem, which says that (10) has a unique and analytic solution in a finite interval of b around zero. In leading order it reads

$$g_S(x)=\frac{\sin 2\pi x}{\kappa+2-2\cos 2\pi c}b+O(b^2). \qquad (13)$$

It fulfills (11). For $b\to\infty$ the last term dominates and the solution has the form

$$g_S(x)=-x+\frac{n(x)}{2}, \quad \text{with } n(x) \ \text{integer}, \qquad (14)$$

where $n(x)$ cannot be a constant because g_S has to be a periodic function. Thus the hull function has at least one jump. Again the implicit function theorem can be applied for b^{-1} around zero because $\cos 2\pi[x+g_S(x)]=(-1)^{n(x)}\neq 0$. The initial jumps of $n(x)$ will be spread everywhere by the mechanism described above.

In the Tomlinson limit of the FKT model (i.e., $\kappa,b\to\infty$) we can discuss the hull function analytically because we can drop the delay terms of (10). We get the hull function $g_S(x)$ in parametric form:

$$g_S(\tau)=\frac{b}{\kappa}\sin 2\pi\tau, \quad x(\tau)=\tau-g_S(\tau). \qquad (15)$$

It is uniquely defined as long as $b<\kappa/(2\pi)$. For $b>\kappa/(2\pi)$ three different values of g_S are possible, at least around $x=0$. The additional two values correspond to a metastable state and an unstable saddle of a single Tomlinson oscillator (see Fig. 3). Thus they are not relevant for the hull function, which describes the ground state. Furthermore, they do not fulfill (11c).

This analysis suggests that the main jump and all additional jumps of the hull function (which are infinitesimally small in the Tomlinson limit) are caused by the appearance

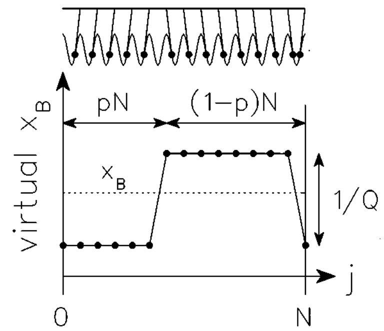

FIG. 4. The first metastable states are kink-antikink pairs. They separate domains with different ground states that are characterized by "virtual" positions x_B of the upper body. The upper part of the figure gives an example for $c=1$ in the Tomlinson limit.

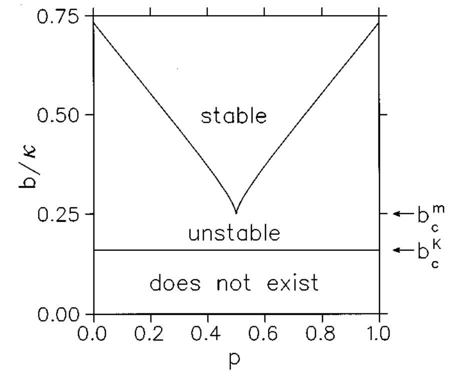

FIG. 5. Phase diagram of the elementary kink-antikink pair for $c=1$ and $N\rightarrow\infty$. The relative portion of one domain is denoted by p.

of *metastable states*. In the following subsection we therefore discuss the question: What kind of metastable states appear first and for which values of b?

B. Metastable states

For small values of b the corrugation is weak and the ground state is still the only stationary stable state. If b is larger than a critical value b_c^K, additional stationary states emerge that have the following properties. They violate condition (8). The matrix $\partial^2 V/\partial\xi_i\partial\xi_j$ is positive definite, which means that these states are stable against infinitesimal small disturbances in ξ_j, $j=1,\ldots,N$. But they may be still unstable against infinitesimal small perturbations, which includes also disturbances in x_B. If b exceeds a further threshold $b_c^m \geqslant b_c^K$, the first of these states become stable.

The first metastable state will not be very different from the ground state. It can be described by the ground state plus a *defect*. But what kind of defect? Naively, one might expect a defect caused by a single hopping of one particle to its neighboring potential well. For the FK model it is known that this is not the case.[16] The elementary defect in the FK model and in the FKT model too — as we will see below — is a *phase kink* that separates two domains with ground states corresponding to different phases x_B defined by (12) (see Fig. 4). The phase of each domain is a kind of "virtual" body position that would be the real position if the other domain did not exist. In the FK model such a phase kink is a localized deviation from the ground state, which means that the kink energy does not depend on the size N of the system if N is much larger than the size of the kink. On the other hand, in the FKT model the energy of such a defect scales with N because of the *nonlocal* coupling of each particle via the upper body. The nonlocality is expressed by condition (5b), which means that the real position x_B is the average over the virtual ones weighted by the domain sizes (see Fig. 4). Thus the difference between the real x_B and the virtual x_B shifts *each* particle out of its ground-state position even if it is far away from the kink.

Another consequence of the nonlocal coupling is that we cannot treat an infinitely extended FKT model because the ratio of the domain sizes would not be defined. Thus we consider a very large but finite system. Because of the periodic boundaries, the numbers of kinks and antikinks have to be equal.

The above-mentioned defect of one particle hopping into the neighboring potential well corresponds to a pair of a kink and an antikink that are as close together as possible. In the following we argue that the first metastable state consists of a pair of a kink and an antikink that are as far away as possible, not because of the usual exponentially decreasing kink-antikink interaction but because of the nonlocality. The difference between the virtual values of x_B of the domain states is $1/Q$.

First we treat the Tomlinson limit, where the kink-antikink interaction disappears because of the absence of the nearest-neighbor interaction. For $b>\kappa/(2\pi)$ and x_B fixed, each Tomlinson oscillator develops additional stationary states because the hull function $g_S(x)$ defined by (15) loses its uniqueness. One of these additional states is metastable for x_B fixed (see Fig. 4). Nevertheless, for b just above $\kappa/(2\pi)$ any state other than the ground state that fulfills the nonlocality condition (5b) is still unstable when x_B is free. In order to see this the most commensurate case (i.e., $c=1$) is treated in Appendix A. It turns out that the first metastable kink-antikink state (see Fig. 4) is indeed that one with equally sized domains (see Fig. 5). It appears for $b>\kappa/4$. Thus

$$b_c^m = \frac{\kappa}{4}, \quad \text{for } c=1. \tag{16}$$

This threshold also holds in general, not only in the Tomlinson limit, because the nearest-neighbor interaction only leads to a finite kink size, but does not change the domain states.

For other values of c we have found numerically that the state with equally sized domains is always the first metastable state. It has the following properties: (i) $x_B \bmod (1/Q)=0$. (ii) All ξ_j's fulfill (7). (iii) All ξ_j's fulfill (8) except for those for which the support of their leaf spring (see Fig. 1) is directly above a maximum of the external potential. The displacement ξ_j is positive in one domain and negative in the other. Thus in one domain every Qth particle violates (8).

In the incommensurate case metastable states appear beyond the point of breaking of analyticity, i.e., $b_c^m \geqslant b_c^S$. Numerically we have some evidence that $b_c^m = b_c^S$ always holds, as in the FK model.[8]

IV. STATIC FRICTION

Before investigating the static friction we have to clarify the meaning of static friction in deterministic zero-temperature models, such as the FKT model. We do this from the point of view of nonlinear dynamics.

A. Definition of static friction

From the phenomenological point of view the static friction F_S is defined as the smallest driving force F that initiates sliding. That is, any force F below F_S does not lead to a relative motion of the surfaces. Thus, the static friction is defined by the *boundaries* of F for which the stationary, motionless *state* is *stable*. Therefore the static friction depends on the internal state of the real contact area between the sliding surfaces, which in the FKT model is determined by the configuration of the N particles describing the surface atoms of the upper body (see Fig. 1). Since different states may have different stability boundaries the static friction is in general not uniquely defined. It will depend on the *history* of the friction system, a well-known experimental fact. For example, it was found[15,17] that the static friction increases with the sticking duration, i.e., the time during which the sliding surfaces do not move (at least not on a macroscopic level).

In view of the nonuniqueness of the static friction the question arises: Is a sound definition of static friction possible that does not depend on the history of the total friction system? The answer to this question is positive and the appropriate definition reads: *The static friction F_S is the smallest driving force above which no stable stationary state exists*. This definition is very similar to the definition of the depinning force in models describing the pinning-depinning transition of charge-density waves or interacting vortices in type-II superconductors. In these models the dynamics is usually treated in the overdamped limit, which has the following consequences. Assuming we start with a metastable state and slowly increase F, the state follows F adiabatically until a certain value is reached where it annihilates with an unstable state in a saddle-node bifurcation. Thus the system depins locally and some degrees of freedom start to move. In the case of overdamped dynamics the system will be trapped by the next relative minimum of the energy surface in configuration space. Thus for a slowly increasing driving force F the system will follow a sequence of depinning events where it locally relaxes into another pinned state. Eventually the system globally depins. This happens at least when the last state disappears.

Applied to friction we see that the above definition of the static friction makes sense in the absence of inertia effects both in the internal degrees of freedom and in the macroscopic sliding body. It is also independent of the history of the friction system. The local reconfigurations may be interpreted as *microslips*[17] that do not lead to sliding on a macroscopic scale. It must, however, be realized that the study of a massless sliding body is somewhat academic, and a discussion of inertia effects will be crucial for a realistic treatment of static friction. Here we emphasize the main difference between models for pinning-depinning transitions, such as the FK model, and models like the FKT model, namely, the *existence of a macroscopic sliding mass that interacts directly with many or even all internal degrees of freedom*, which is also responsible for the *nonlocal* coupling of the internal degrees of freedom. For finite inertia we expect that an unstable state does not evolve into another stable state but rather leads to global sliding. Nevertheless, F_S gives an upper bound for the actual static friction. It is calculated in the next subsection. The static friction in the more realistic case of finite inertia will be discussed elsewhere in the context of stick-slip motion.

B. Static friction of the FKT model

In the previous subsection we have defined the maximum static friction F_S as the driving force F where the last stationary state disappears. The stationary states are the solutions of

$$\begin{aligned} 0 &= -\partial_{\xi_j} V \\ &= \xi_{j+1} + \xi_{j-1} - (2+\kappa)\xi_j + b\ \sin 2\pi(x_B + cj + \xi_j), \end{aligned} \tag{17a}$$

$$0 = -\partial_{x_B} V = \kappa \sum_{j=1}^{N} \xi_j + F. \tag{17b}$$

Without solving (17) it is possible to give an overall upper bound $F_S^{\max}$ for the static friction F_S. Taking the sum over (17a) and using (17b) we get

$$F = -b \sum_{j=1}^{N} \sin 2\pi(x_B + cj + \xi_j), \tag{18}$$

from which it immediately follows that $|F|$ is always smaller than

$$F_S^{\max} = Nb. \tag{19}$$

Starting with a stable, stationary state of the FKT model without driving, what happens if F is quasistatically switched on? First, x_j and x_B will change adiabatically, i.e., they are smooth functions of F. Eventually F will reach a value — the depinning force — where the state annihilates with an unstable stationary state in a saddle-node bifurcation. From physical intuition and from our numerical studies we are convinced that *the ground state of the FKT model has the largest depinning force, which therefore defines the maximal static friction force F_S*. We are able to prove this conjecture only for $c=1$ (see Appendix B), but it is consistent with the above-mentioned experimental observations that the static friction always increases with the sticking time. At the beginning of sticking, just after a global sliding event, the contact area will be in a metastable state. On a large time scale where thermal agitation becomes important, the system will

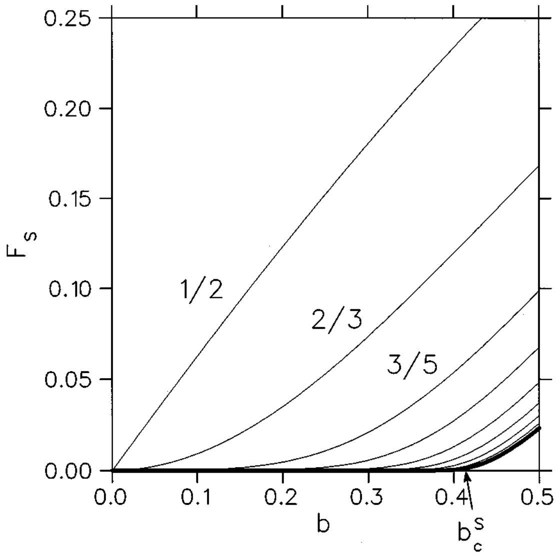

FIG. 6. Static friction F_S as a function of b for $\kappa=1$ and for a sequence of rational values of c (thin lines), which converges to the golden mean $(\sqrt{5}-1)/2$ (thick line).

overcome the barrier and move into a more stable state. By repetition of this process it will eventually reach the ground state.

For $c=1$ and $c=1/2$ we are able to calculate F_S analytically (see Appendix B). For other rational values of c we have calculated F_S numerically. We find the following properties: (i) The maximal static friction F_S as a function of b increases strictly monotonically. (ii) Near zero it scales like

$$F_S \sim b^Q. \tag{20}$$

(iii) For $b\rightarrow\infty$ it approaches $F_S^{\max}$. (iv) For fixed values of b it decreases with decreasing commensurability of c. More precisely: If we organize the rational numbers in a Farey tree,[18] we find that the static friction of some rational value of c is less than the static friction of the parents of this rational number in the Farey tree.

Figure 6 shows $F_S(b)$ for a sequence of rational values of c, which approaches the golden mean $(\sqrt{5}-1)/2$. We see that the sequence of curves converges to a curve with a singularity at the point of breaking of analyticity b_c^S. For $b<b_c^S$ the static friction F_S is exactly zero because the analyticity of the hull function (9) makes it possible to shift the surface atoms of the upper body smoothly over the corrugated surface of the lower body. Thus a Goldstone mode exists and no force is needed for sliding. As static friction and the breaking of analyticity always appear together, we change the meaning of b_c^S. In the following b_c^S denotes the threshold above which the static friction is not zero. In the commensurate case b_c^S is equal to zero.

For $b>b_c^S$, F_S increases strictly monotonically with b. Numerically we find a power law near b_c^S:

$$F_S \sim (b-b_c^S)^\alpha \quad \text{with} \quad \alpha\approx 2. \tag{21}$$

This behavior of F_S is similar to what is found for the depinning force of the ground state of the FK model,[19] except that for the FK model $\alpha\approx 3$. We have checked that in the FKT model the exponent α remains roughly 2 for values of κ down to 0.01. Thus $\alpha(\kappa\rightarrow 0)$ is possibly not continuous at $\kappa=0$.

V. KINETIC FRICTION IN THE QUASISTATIC LIMIT

In this section we analyze the case of vanishing kinetic friction in the quasistatic limit, i.e., sliding velocity $v\rightarrow 0$. The kinetic friction for arbitrary sliding velocities will be calculated elsewhere.

The kinetic friction is the lateral force that is necessary to keep the upper body at a constant velocity v. Thus, the block position x_B is the control parameter contrary to Secs. III and IV where the applied force F was the control parameter.

Quasistatic sliding gives the system enough time to relax into a stable state after an infinitesimal change of x_B. The stationary states, which are solutions of (17a), depend on x_B. From (17b) follows the lateral force

$$F(x_B) = -\kappa \sum_{j=1}^{N} \xi_j(x_B), \tag{22}$$

which is necessary to keep the upper body at position x_B. In the field of nanotribology[2] this lateral force is often called friction force (for example, in the term ‘‘friction force microscopy’’) even though it is not of dissipative character as we will see below. Kinetic friction has to be defined from the *work* that is necessary to slide two interacting surfaces over a finite distance. Thus the kinetic friction F_K is the *averaged lateral force*, i.e.,

$$F_K = -\lim_{x_B\rightarrow\infty} \frac{\kappa}{x_B} \int_0^{x_B} \sum_{j=1}^{N} \xi_j(x)\,dx. \tag{23}$$

As already mentioned in the Introduction, frictionless sliding has attracted some attention in the literature. We emphasize that zero friction for a *finite* velocity is not possible in open systems. The kinetic friction may vanish only for sliding velocity $v\rightarrow 0$. Frictionless sliding simply means that Coulomb's law of constant kinetic friction is replaced by some other (e.g., viscous) friction law where the kinetic friction vanishes for $v\rightarrow 0$.

What is the condition for vanishing kinetic friction in the quasistatic limit? The answer is this: The state of the system must follow the quasistatic change of x_B adiabatically. In this case the ξ_j's are functions of x_B. Thus the potential energy (1) with $F\equiv 0$ becomes a continuous periodic function of x_B, i.e.,

$$\tilde{V}(x_B) \equiv V[\xi_1(x_B), \ldots, \xi_N(x_B), x_B].$$

Using (17) we get for the lateral force (22),

$$F(x_B) = \partial_{x_B} V = \frac{d\tilde{V}}{dx_B},$$

which is a conservative force oscillating around zero. Its average is zero, i.e., $F_K=0$.

As long as b is small there exists only one solution of (17a) for any value of x_B. It is given by the same hull function g_S introduced in Sec. III A in order to characterize the

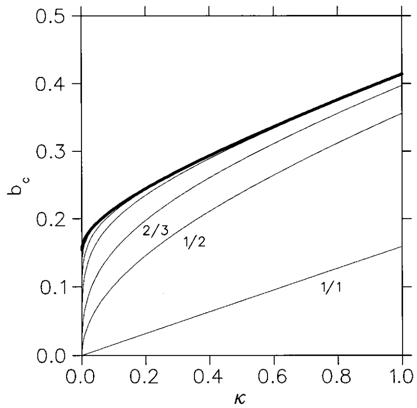

FIG. 7. The threshold b_c^K as a function of κ for a sequence of rational values of c (thin lines), which converges to the golden mean $(\sqrt{5}-1)/2$ (thick line).

ground state (9) of the undriven system even in the commensurate case. The only difference is that now x_B is arbitrary. For $b>b_c^K$ additional stationary states appear as already noted in Sec. III B. The reason is that the hull function g_S is no longer uniquely defined because the solutions of (10) develop loops at values of x that are integer multiples of $1/Q$. The largest loop appears at $x=0$ (see also Fig. 3). The loops correspond to bistability intervals that are bounded by saddle-node bifurcations. When we start with some state, the quasistatic change of x_B moves the state adiabatically until a saddle-node bifurcation is reached. At that point the system has to rearrange itself into a new metastable state. During this rearrangement the particles have to move over a finite distance where they dissipate the energy, which is determined by the difference between the potential energy before and after the rearrangement. Thus $F_K \neq 0$ for $b>b_c^K$. As additional states and kinetic friction in the quasistatic limit always occur together, b_c^K also denotes the threshold below which the kinetic friction vanishes for $v \to 0$.

For $c=1$ and 1/2 we are able to calculate b_c^K analytically (see Appendix C). For other values of c this is possible only numerically. Figure 7 shows numerical results of b_c^K as a function of κ for a sequence of rational values of c approaching the golden mean. We find the following properties: (i) b_c^K as a function of κ increases strictly monotonic. (ii) Near zero it scales as

$$b_c^K \sim \kappa^{1/Q}. \tag{24}$$

(iii) In the Tomlinson limit $\kappa \to \infty$ it approaches $\kappa/(2\pi)$. (iv) For fixed values of κ it increases with decreasing commensurability of c.

In the incommensurate limit b_c^K becomes finite in the limit $\kappa \to 0$. The value $b_c^K(\kappa \to 0)$ is ≈ 0.154, which cannot be distinguished numerically from the value of the point of breaking of analyticity of the FK model for the golden mean.[19] Thus $b_c^K(\kappa \to 0) = b_c^K(\kappa = 0)$. Numerically we find that b_c^K scales near $\kappa = 0$ as

$$b_c^K - b_c^K(0) \sim \kappa^\beta \quad \text{with} \quad \beta \approx \tfrac{1}{2}. \tag{25}$$

In the incommensurate case the breaking of analyticity of the hull function corresponds to the appearance of loops in the solution of (10). Thus, $b_c^K = b_c^S$, which is confirmed by our numerical results. Therefore both static friction and kinetic friction in the quasistatic limit are zero. In the commensurate case, on the other hand, zero kinetic friction does not imply zero static friction. In fact, F_S is always unequal to zero.

VI. CONCLUSION

In this paper we have introduced a simple model of wearless friction, the Frenkel-Kontorova-Tomlinson (FKT) model (see Fig. 1), a combination of the Frenkel-Kontorova (FK) model and the Tomlinson model. Here we have investigated only the static properties of the FKT model. The behavior of the system strongly depends on (i) the strength b of the interaction between the sliding surfaces and (ii) the commensurability of the surface lattices. There are three threshold values of b at which the behavior changes qualitatively.

The first threshold is denoted by b_c^S. Below b_c^S the static friction is zero whereas above b_c^S it increases like a power law and approaches $F_S^{\max} = bN$ in the asymptotic limit. In the commensurate case, where the ratio c of the lattice constants of both sliding surfaces is rational, b_c^S is zero. The exponent of the power law is given by the denominator of c. In the incommensurate case, b_c^S is finite and increases with the ratio κ of the stiffnesses of the leaf and coil springs (see Fig. 1). For the golden mean the exponent is roughly 2.

For b below the second threshold denoted by b_c^K, the kinetic friction F_K is zero in the limit of quasistatic sliding (i.e., sliding velocity $v \to 0$). That is, for $b<b_c^K$ the kinetic friction behaves similarly to viscous friction. For $b>b_c^K$ Tomlinson's basic dissipation mechanism leads to a finite kinetic friction. Therefore b_c^K is also the threshold above which additional stationary states appear that are stationary for fixed relative positions of the sliding bodies. The threshold b_c^K increases with κ and is always larger than zero. Therefore, in the commensurate case vanishing kinetic friction does not imply vanishing static friction. The FKT model for $b>b_c^K$ is an example of a dry-friction system that dynamically behaves like a viscous fluid under shear even though the static friction is not zero. This is a generic behavior that strongly violates Coulomb's third law.

The third threshold, denoted by b_c^m, is important for the precise meaning of the maximal static friction F_S. Below this threshold the ground state of the undriven FKT model is the only stable state. For $b>b_c^m$ additional metastable states appear. The first metastable state is characterized by equally sized domains. The domain states are almost the ground state but for different virtual positions of the sliding bodies (for an example, see Fig. 5). The bulk domain states differ from the exact ground state because the real position is the average of the virtual ones. In the commensurate case the gap in the energy between the first metastable state and the ground state is an *extensive* quantity, i.e., it is proportional to the number of particles. This is a consequence of the *nonlocal* character of the FKT model.

Since the static friction is the force that is necessary to start sliding, it depends on the state of the system. Therefore static friction is not uniquely defined for $b>b_c^m$, but the function $F_S(b)$ introduced in Sec. IV gives an upper limit of the actual static friction. It is defined as the smallest force above which there exists no stable state. We have seen that F_S is given by the force required to depin the model from the ground state.

The relation between these thresholds depends on whether c is rational or irrational. For the commensurate case the relation is

$$0=b_c^S<b_c^K<b_c^m. \tag{26}$$

For the incommensurate case it is

$$0<b_c^S=b_c^K=b_c^m. \tag{27}$$

Concerning the static properties of the FKT model there remain many open questions to be investigated. From the mathematical point of view, a number of conjectures has been presented in this paper for which we have strong numerical evidence but no rigorous proof. For example, it is evident from physical intuition that the ground state has the largest depinning force. This has been found also in more complex systems.[20] It would be desirable to have a proof of this conjecture at least for a certain class of models.

Although the FKT model is a very simplified model even for atomically flat surfaces, we believe that it is able to mimic some of the qualitative behavior of real systems. The FKT model has the potential to become a prototypical model for dry friction of atomically flat surfaces, such as the FK model, for the commensurate-incommensurate transition and charge-density waves.

The FKT model can be extended in various directions. An important one would be the introduction of quenched randomness due to unavoidable surface impurities because in FK-like models it may destroy the frictionless state in the incommensurate case.[21]

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APPENDIX A: THE FIRST METASTABLE STATE IN THE TOMLINSON LIMIT FOR $c=1$

For the Tomlinson limit (i.e., $\kappa,b\to\infty$ but b/κ finite) of the undriven FKT model we drop the first two terms of the potential (1). Stationary states are solutions of

$$\partial_{x_j}V=\kappa\xi_j-b\sin 2\pi(x_B+cj+\xi_j)=0 \tag{A1}$$

and (5b). A stationary state is stable if the second derivative of the potential DV is a positive definite matrix. It reads

$$DV\equiv\begin{pmatrix} D_1 & 0 & \dots & 0 & -\kappa \\ 0 & D_2 & \dots & 0 & -\kappa \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & D_N & -\kappa \\ -\kappa & -\kappa & \dots & -\kappa & N\kappa \end{pmatrix}, \tag{A2}$$

where

$$D_j=\kappa+C_j \quad \text{with} \quad C_j=-2\pi b\cos 2\pi(x_B+cj+\xi_j). \tag{A3}$$

It is positive definite if all D_j's and $\det DV$ are positive. After some algebraic operations one finds

$$\det DV=\kappa\left(\prod_{j=1}^{N}D_j\right)\sum_{j=1}^{N}\frac{C_j}{D_j}. \tag{A4}$$

Thus the stability conditions read

$$\sum_{j=1}^{N}\frac{C_j}{D_j}>0 \quad \text{and} \quad D_j>0, \quad j=1,\dots,N. \tag{A5}$$

A sufficient condition for stability is

$$C_j>0, \quad j=1,\dots,N. \tag{A6}$$

For the case $c=1$ we investigate the existence and stability of solutions containing a kink and an antikink in more detail. The solution has two domains where ξ is uniform in each domain. There are $N_\pm$ particles with $\xi_\pm$ fulfilling (A1) with $N_++N_-=N$. The definition $p=N_+/N$ measures the extent of the plus domain relative to the total extent of the system. Because of (5b) it has to fulfill

$$p\xi_++(1-p)\xi_-=0. \tag{A7}$$

The solution is stable if $pC_+/D_++(1-p)C_-/D_->0$ and $D_\pm>0$. Eqs. (A1), (A7), and

$$p\frac{C_+}{D_+}+(1-p)\frac{C_-}{D_-}=0 \tag{A8}$$

define implicitly b/κ as an even function of $p-1/2$. The numerical solution is shown in Fig. 5. The minimum at $p=1/2$ can be calculated analytically because (A7) implies $\xi_-=-\xi_+$. Furthermore, $x_B=0$ because of (A1) and therefore $C_\pm=-2\pi b\cos 2\pi\xi_+$. Thus (A8) reduces to $C_\pm=0$, which implies $\xi_+=1/4$. With (A1) we get $b_c^m=\kappa/4$.

APPENDIX B: F_S FOR $c=1$ AND $c=1/2$

In accordance with our conjecture that the static friction F_S is given by the depinning force of the ground state, we solve the delay equation (10) for the hull function g_S. Using (9) and (17b) we get

$$F(x_B)=-\kappa\sum_{j=1}^{N}g_S(x_B+cj). \tag{B1}$$

The static friction F_S is determined by the maximum of $F(x_B)$, which can be obtained by equating the extrema.

First we calculate F_S for $c=1$. Because of the periodicity of g_S the delay equation turns into an algebraic equation

$$0=-\kappa g_S(x)+b\sin 2\pi[x+g_S(x)]. \tag{B2}$$

For F we get

$$F(x_B)=-\kappa N g_S(x_B)=-bN\sin 2\pi[x+g_S(x)]. \tag{B3}$$

The extrema of F are also extrema of g_S. From (B2) follows

$$\frac{dg_S}{dx}=\frac{2\pi b\cos 2\pi[x+g_S(x)]}{\kappa-2\pi b\cos 2\pi[x+g_S(x)]}. \tag{B4}$$

The extrema are implicitly defined by $x+g_S=n/2+1/4$, n integer, which leads to

$$F_S=bN. \tag{B5}$$

Thus F_S is equal to the overall upper bound $F_S^{\max}$, which proves our conjecture that the ground state has the largest depinning force.

For the case $c=1/2$ we introduce $g_1(x)\equiv g_S(x)$ and $g_2(x)\equiv g_S(x+1/2)$. In accordance with the symmetries (11a) the delay equation (10) turns into a system of two coupled algebraic equations,

$$0=2g_2(x)-(2+\kappa)g_1(x)+b\sin 2\pi[x+g_1(x)],$$
$$0=2g_1(x)-(2+\kappa)g_2(x)-b\sin 2\pi[x+g_2(x)]. \tag{B6}$$

For F we get

$$F(x_B)=-\frac{\kappa N}{2}[g_1(x_B)+g_2(x_B)]. \tag{B7}$$

It is not possible to give an analytic expression of F_S as an explicit function of b. But we are able to express $F_S(b)$ in parametric form, i.e., $F_S(D)$ and $b(D)$, where the parameter D is defined by

$$D=g_1-g_2. \tag{B8}$$

Together with (B7) we can rewrite (B6):

$$0=\frac{F}{N}+b\cos 2\pi\left(x-\frac{F}{\kappa N}\right)\sin\pi D,$$

$$0=-\left(2+\frac{\kappa}{2}\right)D+b\sin 2\pi\left(x-\frac{F}{\kappa N}\right)\cos\pi D. \tag{B9}$$

Eliminating x we get

$$\frac{F}{F_S^{\max}}=\pm\sin\pi D\sqrt{1-\left(\frac{(4+\kappa)D}{2b\cos\pi D}\right)^2}. \tag{B10}$$

In order to get the extrema of $F(x_B)$ we differentiate (B9) in x. Using $dF/dx\equiv 0$, eliminating dD/dx and $x-F/(\kappa N)$ we get

$$b=\frac{4+\kappa}{2\pi\cos^2\pi D}\sqrt{(\pi D+\sin\pi D\cos\pi D)\pi D}. \tag{B11}$$

Equations (B11) and (B10) define $F_S(b)$ parametrically. Expansions into Taylor series around $D=0$ and $D=1/2$ yield

$$\frac{F}{F_S^{\max}}=\frac{\pi}{4+\kappa}b+O(b^2), \tag{B12}$$

and

$$\frac{F}{F_S^{\max}}=1-\frac{4+\kappa}{4}b^{-1}+O(b^{-2}), \tag{B13}$$

respectively.

APPENDIX C: b_c^K FOR $c=1$ AND $c=1/2$

Loops appear in the solutions of (10) when the slope of $g_S(x)$ becomes infinite. For $c=1$ the delay equation (10) turns into the algebraic equation (B2). Near $x=0$ we make the ansatz

$$g_S(x)=g'x+O(x^2), \tag{C1}$$

which yields

$$0=[-\kappa g'+2\pi b(1+g')]x+O(x^2). \tag{C2}$$

Equating the coefficient of x^1 equal to zero we get

$$g'=\frac{2\pi b}{\kappa-2\pi b}. \tag{C3}$$

The slope of $g_S(x)$ becomes infinite at $x=0$ for b equal to

$$b_c^K=\frac{\kappa}{2\pi}. \tag{C4}$$

For the case $c=1/2$ the delay equation (10) turns into the system of algebraic equations (B6) for $g_1(x)\equiv g_S(x)$ and $g_2(x)\equiv g_S(x+1/2)$. Again we expand g_1 and g_2 in Taylor series:

$$g_i=g_i'x+O(x^2), \quad i=1,2. \tag{C5}$$

Inserting this ansatz into (B6) and equating the coefficient of x^1 equal to zero leads to

$$(2+\kappa-2\pi b)g_1'-2g_2'=2\pi b$$

$$-2g_1'+(2+\kappa+2\pi b)g_2'=-2\pi b. \tag{C6}$$

The solution is

$$g_{1,2}=\frac{2\pi b(2\pi b\pm\kappa)}{(4+\kappa)\kappa-(2\pi b)^2}. \tag{C7}$$

Thus the slope of g_S becomes infinite at $x=0$ and $x=1/2$ for b equal to

$$b_c^K=\frac{\sqrt{(4+\kappa)\kappa}}{2\pi}. \tag{C8}$$

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