Friction and second-order phase transitions

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(Received 24 July 2003; revised manuscript received 29 July 2004; published 25 October 2004)

A microscopic model is studied numerically to describe wearless dry friction without thermal fluctuations between atomically flat contact interfaces. The analysis is based on a double-chain model with a Lennard-Jones interaction between the chains which are the respective upper flexible monolayers of the rigid bulk systems. Whereas below a critical interaction strength ϵ_c the system exhibits a frictionless state, it offers static friction above ϵ_c. Introducing an appropriate order parameter function we demonstrate the analogy of the critical behavior to a phase transition of second order. The order parameter is related to a hull function describing uniquely the incommensurate ground state of the model. The breakdown of analyticity of the hull function is identified with the phase transition. Critical exponents are calculated and the validity of finite-size scaling is displayed.

DOI: 10.1103/PhysRevE.70.046113 PACS number(s): 68.35.Af, 81.40.Pq, 64.60.−i, 64.70.Rh

I. INTRODUCTION

The study of friction is a long-standing problem in physics which has encountered renewed interest recently in different context [1–5]. There are several ways to analyze frictional phenomena. Based on experimental observations the frictional behavior can be characterized by an empirical formula such as the Coulomb-Amonton laws [6]. Macroscopically, one can usually observe that two solids are slid past each other under suffering wear. But wear seems not to be necessary for the occurrence of friction. In the last few years, technological developments have made it possible to study wearless dry friction between atomically flat contact interfaces experimentally (nanotribology) [6–8]. These experiments on a nanoscale have stimulated theoretical efforts in investigating friction phenomena within microscopic models [9–17]. Recently [18] friction has been studied in carbon nanotubes based on experimental observations with the transmission electron microscope technique in multiwall nanotubes [19]. Obviously, the dissipative nature of friction is a typical nonequilibrium problem. Based on that observation the Langevin description seems to be a convenient tool on a mesoscopic scale and at finite temperatures [20–22] to attack the problem. Contrary to that approach we analyze a microscopic model, in which the wearless dry friction between two atomic flat layers can be explained in terms of the Aubry transition using a simple driven many-body system on a lattice with an appropriate interaction. Based on an incommensurate structure the Aubry transition or the analyticity breaking transition is equivalent to the breakup of tori in the standard map, which can be related to a transition between the so-called superlubricity and the friction regime at a critical value of the interaction strength.

One of the simplest microscopic systems is given by a discrete version of the well-known Frenkel-Kontorova (FK) model [23]. That FK model describes harmonically coupled particles on a chain under the influence of an additional periodic potential. It is mainly used to discuss the adsorption of a monolayer on an atomically flat clean substrate surface. In the case of a constant external force, applied to each particle of the chain, this driven FK model can also be used as a simple model for wearless friction [9–11]. Notice that several physical phenomena such as the motion of dislocations in crystals [24], the commensurate-incommensurate transition [25,26], and charge-density waves (CDW's) [27,28] could be investigated with modified FK models. The FK model is apparently a good starting point for constructing more complex friction models on the atomic level. Thus, a natural extension of the FK model consists of replacing the rigid substrate (hard body) by a deformable substrate monolayer pinned to a solid (soft body). Such a more refined microscopical model of friction was introduced by Matsukawa and Fukuyama [12,13]. They considered a one-dimensional model composed of two deformable interacting harmonic chains, where each particle of the lower chain is harmonically pinned to a rigid solid. The static and kinetic properties of this two-chain model of friction were analyzed in great detail in [14,15]. The mentioned models [12–15] are involved in a larger class of systems, classified as the Frenkel-Kontorova-Tomlinson (FKT) model. The FKT model, introduced by Weiss and Elmer [16,17], describes wearless dry friction between atomically flat bulk materials where the adsorbated monolayer is replaced by a substrate. It is likewise a one-dimensional lattice model for a soft upper body sliding on a hard lower body. In contrast to the two-chain model, the feature of the FKT model is a harmonic coupling of each particle of the adsorbate monolayer to an upper sliding mass, assumed to be a macroscopic one, whose position, relative to the lower surface, is characterized by the coordinate x_B. Remarkably, in all these one-dimensional microscopic friction models the particles within the chain are allowed to move

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only parallel to the direction of an applied external force. The stationary states for the FK model [29,30] and the FKT models [12–16] in the absence of external forces have been studied in detail using the so-called hull function. One finds a continuous hull function in case of incommensurate chains below a critical strength of the interaction between the chain and substrate. As a consequence, a certain ground state can be continuously transformed into another ground state without cost of energy. Such a behavior is denoted as an unpinned phase related to the superlubricity regime. On the other hand, above the critical interaction strength, the hull function for the incommensurate chains develops an infinite number of discontinuities. Thus, a ground state cannot be smoothly evolved from another ground state.

In the present paper we investigate numerically a more realistic version of the Frenkel-Kontorova-Tomlinson model [16] with a deformable substrate. The two interacting atomic chains are embedded in a two-dimensional space. Both monolayers at the corresponding contact interface are elastically coupled to the underlying rigid bodies. Additionally, we assume a Lennard-Jones-like interaction between the constituents of both chains. This mutual interaction between the double chains is figured as the internal driving force. We demonstrate the existence of a critical coupling strength, above which the system offers friction. Whereas below the critical interaction strength an arbitrary small external force leads to a global sliding motion of both monolayers against each other (denoted as frictionless motion [16]), above the critical interaction both chains are in a locked state; i.e., a finite external force is necessary to overcome the pinned state (friction). The phenomenon is interpreted as a kind of phase transition which is visualized by introducing an appropriate order parameter function. Remarkably, this phase transition is different from a conventional phase transition. This is manifested by the relation of the order parameter to a so-called hull function. This function describes uniquely the ground state of our model. Above the critical interaction strength the hull function changes from an analytical function to nonanalytical one, which was demonstrated in [30]. Thus the transition is characterized by breaking of the analyticity of the hull function and corresponds to the onset of stochasticity in the standard map. Adopting that concept we analyze the model, introduced above, in terms of the hull function. Our main focus is to study the transition by calculating the hull function. We demonstrate numerically the breaking of the analyticity and show that in terms of the order parameter the phenomenon is similar to the behavior at a second-order phase transition. Here we carry forward an idea proposed by Coppersmith and Fisher [27,28]. Different to that approach our analysis is concentrated on the incommensurate ground state. In particular, we calculate critical exponents and demonstrate the validity of scaling properties for finite systems. Notice that the present model class is quite different to the approaches of driven disordered interfaces in contact with the surface of substrates and their critical regimes. The present model deals with ground-state equations offering a transition equivalent to smooth or chaotic orbits in the standard map below and above a critical interaction strength. In that context, the system offers above the critical interaction strength a finite gap in the excitation spectrum for large wavelengths, while the long-wavelength modes of the incommensurate unpinned phase converge to zero. This means that an unpinned incommensurate phase corresponds to zero static friction whereas the pinned incommensurate phase is equivalent to a finite static friction. Remarkably, the hull function and its analytical properties offer only a rather formal view of the mathematical background. Our analysis suggests that the concept of the order parameter is better qualified for understanding the physical mechanism.

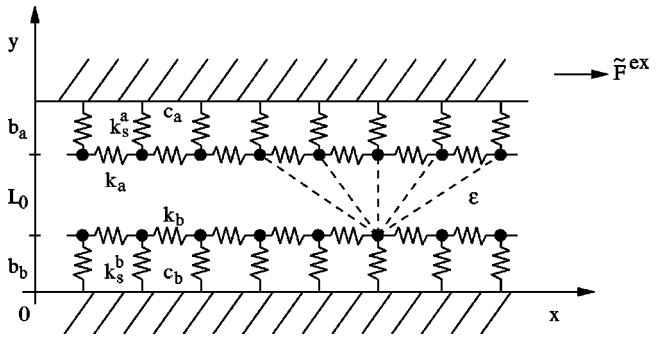

FIG. 1. A schematic picture of the two-dimensional double-chain model. The external force $\tilde{F}^{ex}$ is given by the applied force F^{ex} which acts on each particle of the upper chain times the particle number N_a of the upper chain, where N_a (N_b) is the particle number of the upper (lower) chain.

Notice that another approach is used in [31], however with a special total potential energy relevant for a gold/gold interface. While in [31] the interaction is affected by an external compression, which can lead to friction, we have studied the case that the chains interact under their own adhesive load. Whereas our approach is restricted to a quasi-one-dimensional friction model there exist also calculations in higher dimensions such as [21,32,33]. A transition to a finite static friction was observed in [21] and [32], but the order of the transition was not discussed. The near-commensurate behavior, described in [33], is quite different from the work considered here.

II. MODEL

A. Double-Chain model

Following Matsukawa and Fukuyama [12,13], we introduce the double-chain model as a two-dimensional microscopic lattice model system describing wearless dry friction between two atomically flat solids. Therefore, we consider two deformable atomic chains, denoted as the upper and lower chains. The atoms in each chain are classical particles which are able to perform a two-dimensional movement. Further, we assume a harmonic interaction of the particles within each chain. The interaction between the two chains is supposed to be of Lennard-Jones type. Moreover, both chains are coupled harmonically to an upper or a lower substrate, respectively. The situation we have in mind is depicted in Fig. 1. The external force $\tilde{F}^{ex}$ is pulling the chains apart whereas the mutual interaction is pushing the surface together. The Lennard-Jones potential prevents direct contact of the atoms of the chains. Denoting the two-dimensional

position vectors of the ith particle in the upper or lower chain by $\mathbf{r}_i^a=(x_i^a,y_i^a)$ and $\mathbf{r}_i^b=(x_i^b,y_i^b)$, the equilibrium state is defined by the solutions of

$$0=k_a^x[x_{i-1}^a+x_{i+1}^a-2x_i^a]-k_{sub}^{a_x}[x_i^a-ic_a]+\sum_{j=1}^{N_b}F_{int}^x(x_i^a-x_j^b), \tag{1}$$

$$0=k_a^y[y_{i-1}^a+y_{i+1}^a-2y_i^a]-k_{sub}^{a_y}[y_i^a-(b_b+L_0)]+\sum_{j=1}^{N_b}F_{int}^y(y_i^a-y_j^b), \tag{2}$$

$$0=k_b^x[x_{i-1}^b+x_{i+1}^b-2x_i^b]-k_{sub}^{b_x}[x_i^b-ic_b]+\sum_{j=1}^{N_a}F_{int}^x(x_i^b-x_j^a), \tag{3}$$

$$0=k_b^y[y_{i-1}^b+y_{i+1}^b-2y_i^b]-k_{sub}^{b_y}[y_i^b-b_b]+\sum_{j=1}^{N_a}F_{int}^y(y_i^b-y_j^a), \tag{4}$$

where N_a (N_b) is the particle number and c_a (c_b) is the mean atomic spacing in the x direction of the upper (lower) chain. For a compact representation one can introduce the chain index $I=(a,b)$ relating to the upper and lower chains. k_I^x and k_I^y are the strength of the harmonic interaction force in the chains for the x and y directions. The strength of the coupling of each chain to an upper and a lower substrate is represented by $k_{sub}^{I_x}$ and $k_{sub}^{I_y}$, which determine the rigidity of the chains. A further system parameter is the substrate-substrate distance $L_s=b_a+b_b+L_0$, where b_a (b_b) is the mean atomic spacings in the y direction between the upper (lower) chain and upper (lower) substrates. L_0 denotes the mean distance between the two harmonic chains tuned in a self-consistent manner due to the Lennard-Jones interaction. The interaction force between the upper and lower chains, projected on the x and y axes, can be written as

$$\sum_{j=1}^{N_J}F_{int}^x(x_i^I-x_j^J)=\sum_{j=1}^{N_J}F(r_{ij})\frac{(x_i^I-x_j^J)}{r_{ij}}, \tag{5}$$

$$\sum_{j=1}^{N_J}F_{int}^y(y_i^I-y_j^J)=\sum_{j=1}^{N_J}F(r_{ij})\frac{(y_i^I-y_j^J)}{r_{ij}}, \tag{6}$$

with the chain indices $I=(a,b)$ and $J=(b,a)$ and the distance $r_{ij}=|\mathbf{r}_i^a-\mathbf{r}_j^b|\equiv\sqrt{(x_i^b-x_j^a)^2+(y_i^b-y_j^a)^2}$ relating to the ith atom of the upper (a) and the jth atom of the lower (b) chain. $F(r_{ij})$ can be expressed by the potential $V(r_{ij})$ through $F(r_{ij})=-\partial V(r_{ij})/\partial r_{ij}$. As interaction potential we choose specifically the Lennard-Jones potential

$$V(r_{ij})=4\epsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12}-\left(\frac{\sigma}{r_{ij}}\right)^{6}\right], \tag{7}$$

representing the character of the friction due to the intermolecular forces in the most appropriate way. Here ϵ is the strength of the interaction and σ is a characteristic length scale, by which the minimum of the potential at r_0 in Eq. (7) can be parametrized. It results in $r_0=\sigma 2^{1/6}$.

Our studies are restricted to a region at low temperatures where thermal effects can be neglected. Such a situation is realized experimentally in nanotubes [19]; compare also [18].

B. Numerical method

In this subsection we introduce the numerical method. For solving the two-dimensional double-chain model periodic boundary conditions in both chains are applied:

$$x_i^I=x_{i+N_I}^I-L_I, \tag{8}$$

$$y_i^I=y_{i+N_I}^I, \tag{9}$$

where $I=a,b$ means the chain index and $L_I=N_Ic_I$ is the chain length. Consequently, the system sizes of the upper and lower chains are the same, $L\equiv N_ac_a=N_bc_b$. Hence, the ratio of the two lattice constants (misfit) could be expressed by the particle numbers

$$\alpha=\frac{c_a}{c_b}=\frac{N_b}{N_a}. \tag{10}$$

In that manner the ratio α of the two lattice constants is always a rational number within the numerical realization. The subsequent analysis is based on the concept of the hull function which characterizes the ground state of the underlying model system. Following Aubry [29,30] the incommensurate state is realized by an irrational ratio α between c_a and c_b. The behavior of the system is described by a so-called hull function which will be introduced in the subsequent section. This function loses its mathematical usefulness for rational α. The ground state of the system is an incommensurate one, related to an irrational value α of the two lattice constants. Obviously it is necessary in the numerical implementation to approximate an irrational number through an optimal ratio of two natural numbers. This will be realized by a finite continued-fraction expansion up to a certain order [34,35]:

$$\alpha=a_0+\cfrac{1}{a_1+\cfrac{1}{a_2+\cfrac{1}{\cdots+\cfrac{1}{a_{n-1}+\cfrac{1}{a_n}}}}}. \tag{11}$$

We choose the simplest continued-fraction expansion with $a_0=1$ and $a_1=a_2=\cdots=a_n=1$, so that α could be expressed by the ratios of Fibonacci numbers $F_{n+1}=F_n+F_{n-1}$, where $n=1,2,3,\ldots$ as well as $F_0=1$ and $F_1=1$. Hence,

$$\alpha_n = \frac{F_{n+2}}{F_{n+1}} = \frac{3}{2}, \frac{5}{3}, \frac{8}{5}, \frac{13}{8}, \frac{21}{13}, \frac{34}{21}, \frac{55}{34}, \frac{89}{55}, \frac{144}{89}, \frac{233}{144}, \frac{377}{233}, \frac{610}{377}, \frac{987}{610}, \frac{1597}{987}, \cdots \tag{12}$$

and the irrational limit $\alpha_\infty \equiv \lim_{n\to\infty}(F_{n+2}/F_{n+1}) = 1/2(\sqrt{5}+1)$ of the approximation series (12) is the inverse of the so-called *golden mean*. From the point of view of number theory [35], this is the soonest incommensurable case of the underlying model system, which could be emulated in a systematic way. In our studies we set the lattice constant of the lower chain equal to 1 ($c_b = 1$). Accordingly, the upper mean lattice spacing c_a is equal to α_n and we calculated with the system sizes

$$c_a = \frac{N_b}{N_a} = \frac{89}{55}, \frac{233}{144}, \frac{377}{233}, \frac{610}{377}, \frac{1597}{987}. \tag{13}$$

It should be mentioned that not all ratios of the approximates are "good" irrational number approximations. In order to discuss the essential features of the present model we restrict the wide range of model parameters by setting $k_I^x = k_I^y = 1$, $k_{sub}^{I_x} = k_{sub}^{I_y} = 1$, and $\sigma = 1$. For calculating the stable stationary states we have used a relaxation procedure [15].

III. NUMERICAL RESULTS

A. Hull function

Similarly to the FK model [29] or FKT model [16], the lattice structure of the particle positions in the incommensurate ground state can be uniformly described by a hull function. For examining the lattice structure of the present two-dimensional double-chain model, it is necessary to introduce four hull functions due to two degrees of freedom of the particles in each chain. The two hull functions h_a and h_c of the upper chain are defined as

$$x_i^a = i\, c_a + \phi + h_a(i\, c_a + \phi), \tag{14}$$

$$y_i^a = b_b + L_0 + \phi' + h_c(i\, c_a + \phi'), \tag{15}$$

and the two hull functions h_b and h_d of the lower chain are given by

$$x_i^b = i\, c_b + \psi + h_b(i\, c_b + \psi), \tag{16}$$

$$y_i^b = b_b + \psi' + h_d(i\, c_b + \psi'), \tag{17}$$

where ϕ, ϕ', ψ, and ψ' are constant phases. Note that x_i^a, y_i^a, x_i^b, and y_i^b are the actual positions of the particles in the ground state under the influence of the interaction. For our investigations, it is convenient to set $\phi = \phi' = \psi = \psi' = 0$. The hull functions are periodic and even, which can usually be expressed by

$$h_a(z + c_b) = h_a(z) = -h_a(-z), \quad h_c(z + c_b) = h_c(z) = -h_c(-z), \tag{18}$$

$$h_b(z + c_a) = h_b(z) = -h_b(-z), \quad h_d(z + c_a) = h_d(z) = -h_d(-z). \tag{19}$$

The argument z of h_a and h_c is defined in the range from 0 to c_b, whereas of h_c and h_d it is given from 0 to c_a. Note that the visualization concept of the hull function makes it necessary that the arguments of the just-defined hull functions h_a, h_c or h_b, h_d must be the same, respectively, because the displacements in the x and y directions of all particles in each chain can be assigned to different values of the argument z due to the irrational ratio α of the mean lattice spacing c_a and c_b.

First, we have numerically calculated the ground state of the double-chain model for a fixed ratio $\alpha_n = N_b/N_a$ of particle numbers given by $N_a = 233$ and $N_b = 377$. Several investigations of the FK model [30] and FKT model [16] as well as the two-chain model [15] showed that the ground state depends strongly on the interaction strength ϵ. Therefore, we started the computation for different values of ϵ in the wide range from 0.05 to 0.4. For small values of ϵ up to a certain value ϵ_c we get the result that the periodic hull functions h_a, h_b, h_c, and h_d are analytic—i.e., smooth and continuous. This behavior is illustrated in Fig. 2, where the interaction strength has the value $\epsilon = 0.22$. Furthermore, the stationary state for $\epsilon = 0.22$ is characterized by the mean distance $L_0 = 0.986\ 273$ between the upper and lower chains. Figure 3 shows another numerical calculation of the hull functions for the interaction strength $\epsilon = 0.33$ with the corresponding mean distance $L_0 = 0.959\ 584$. We can observe that the hull functions in Fig. 3 are discrete, which means that they are no longer analytic. This discrete structure is related to jumps, which occur at certain points of the argument z of the hull functions. Now, comparison of Fig. 2 with Fig. 3 shows the phenomenon of breakdown of analyticity, which is due to two significant aspects of the hull functions h_a, h_b, h_c, and h_d for the interaction strengths $\epsilon < \epsilon_c$ and $\epsilon > \epsilon_c$, which defined a certain transition value ϵ_c above which the hull functions are no longer analytic. For a detailed analysis of the threshold ϵ_c we introduced a suitable order parameter in the following part.

Peyrard and Aubry have shown [30] that the breaking of analyticity of the incommensurate ground state of the FK model is characterized by the existence of a largest central gap at half the period of the hull function. The situation in the two-chain model of Matsukawa and Fukuyama [13] is quite different for several elastic parameters. Two simple cases are observed: (i) either h_a or h_b has the largest central gap and (ii) both hull functions do not have the largest central gaps, but two symmetrical gaps with the same size referring to half the period. In Fig. 3 we observe also no largest central gap for all hull functions of the two-dimensional double-chain model. Furthermore, the hull functions show also two symmetrical gaps of the same size referring to half

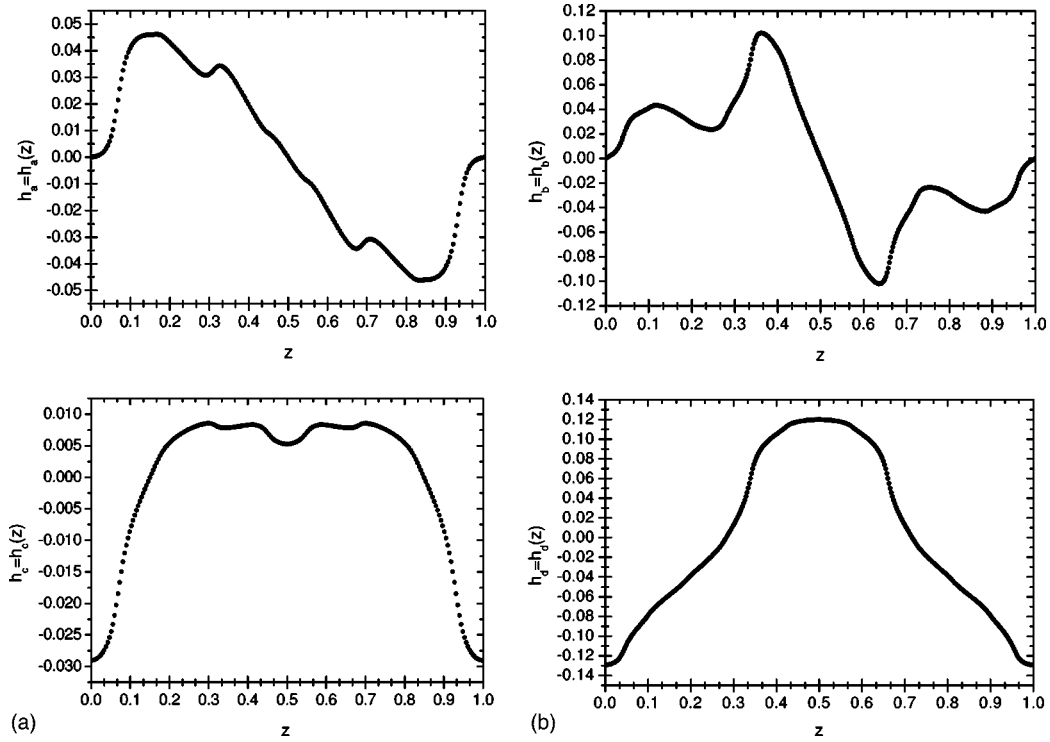

FIG. 2. The hull functions of the ground state plotted for particle numbers $N_a=233$ and $N_b=377$ with interaction strength $\epsilon=0.22$. For a uniform representation all hull functions are renormalized by the mean lattice spacings c_b and c_a, respectively. Therefore, the substitution for the hull function h_a and h_c of the (a) chain is $z\rightarrow z/c_b$, whereas for the hull functions h_b and h_d of the (b) chain it is $z\rightarrow z/c_a$.

the period of the hull function in the whole parameter range analyzed. Up to now we have only investigated the ground-state structure for a fixed system size ($N_a=233$ and $N_b=377$) and a certain range of interaction strength ϵ. Now, we vary the system size of the underlying model which corresponds the different approximation orders of the irrational number through a rational ratio of the particle numbers. Here, we calculated especially the ground-state structure for

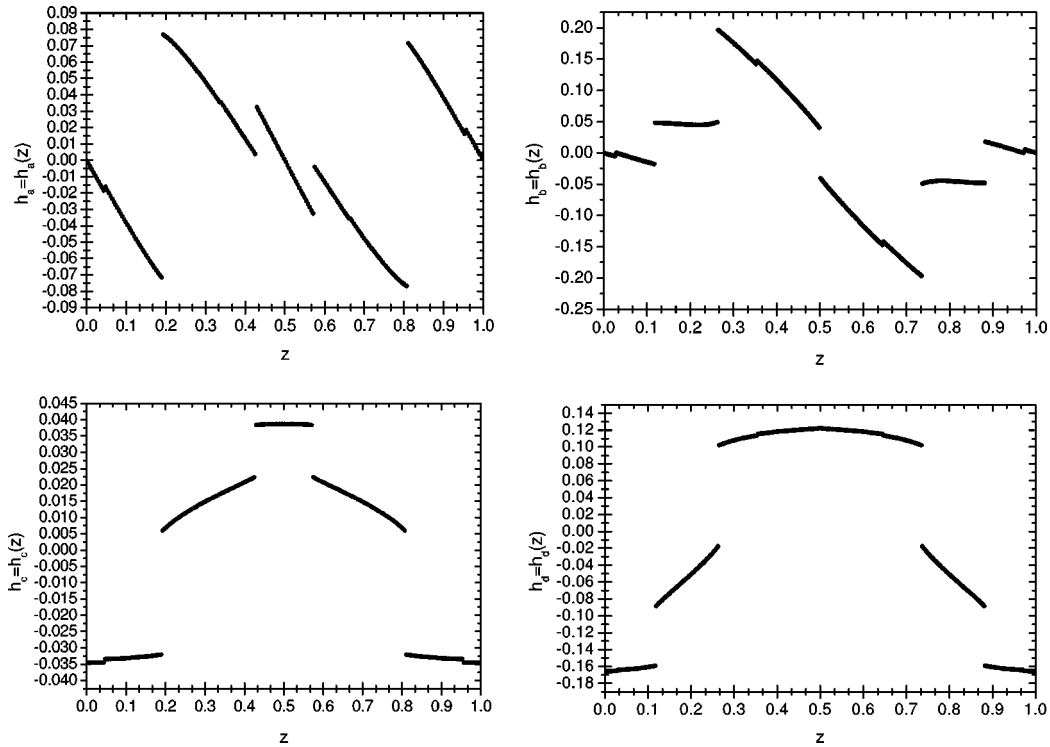

FIG. 3. Hull functions of the ground state for $\epsilon=0.33$ and particle numbers $N_a=233$ and $N_b=377$.

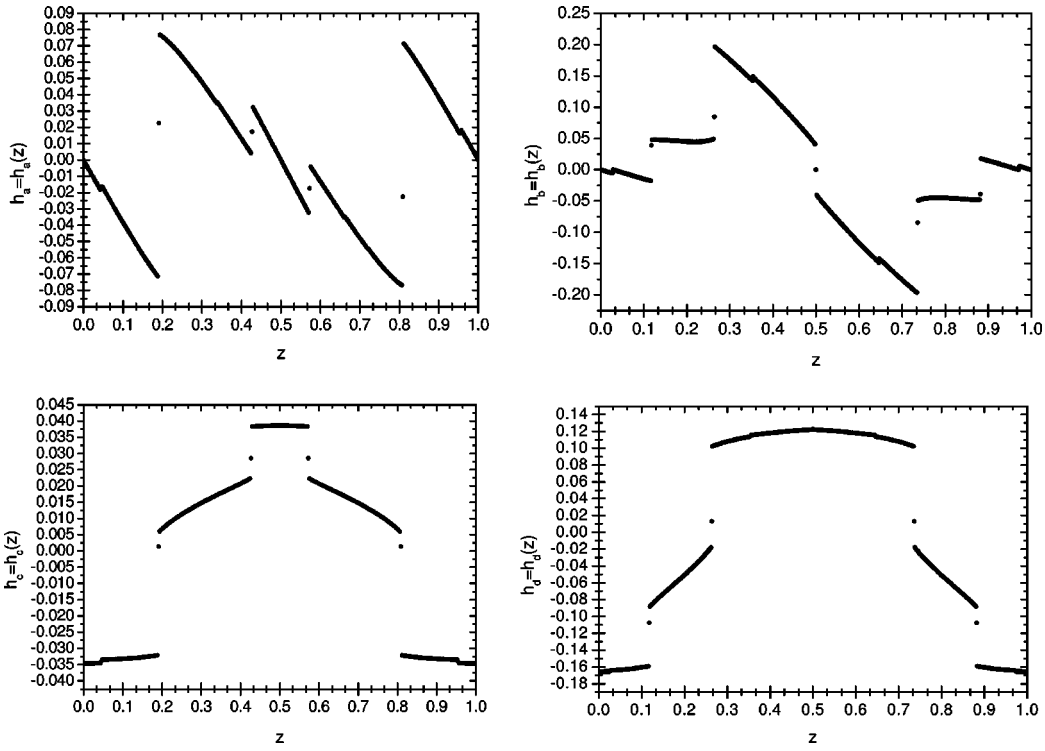

FIG. 4. Artifacts in the hull functions for a bad choice of particle numbers—e.g., given by $N_a=377$ and $N_b=610$—and interaction strength $\epsilon=0.33$.

the ratios $\alpha_n=89/55$, $233/144$, $610/377$, and $1597/987$ in the same range of interaction strength ϵ like above. In particular, we investigated whether there occurs an anomalous behavior in the structure of the hull functions for certain values of ϵ due to the use of a rational ratio instead of an irrational number in the numerical computation. Indeed, Fig. 4 shows such an anomalous behavior of the hull functions for $\epsilon=0.33$ and for the particle numbers $N_a=377$ and 610. In comparison with Fig. 3 we can recognize that the even particle number $N_b=610$ generates a "strange" particle position at half the period $z=0.5$ of h_b in Fig. 4 and other special points. Such not fully understandable artifacts can be also observed for other ratios α_n and interaction strength ϵ. On the assumption that the main structure of the hull function is conserved in course of the approach $\alpha_n \to \alpha_\infty$ for a fixed interaction parameter ϵ (at least above a sufficiently large n) we conclude that only more details can be observed with decreasing difference $|\alpha_n-\alpha_\infty|$. Thus, a change of the fine structure—i.e., the creation of new small gaps may be possible—but larger gaps observed first for small n are fixed. The appearance of pointlike artifacts in some gaps for a given interaction energy ϵ can be observed for some values of n. However, there is neither a stabilization of this phenomenon above a sufficiently large n nor a change of the main structure of the hull function related to the appearance of these artifacts during a systematic approach $\alpha_n \to \infty$ [36].

Relating to the stationary state, Fig. 5(a) shows the mean distance L_0 between the upper and lower chains as a function of strength ϵ of the interaction force, which was calculated for particle numbers $N_a=233$ and $N_b=377$. The plot in Fig. 5(a) shows the computation of L_0 for ϵ in range from 0.05 to 0.45 and Fig. 5(b) shows L_0 in the transition area. Note that the mean distance L_0 is remarkably insensitive to the system size. For the system sizes $\alpha_n=377/233$, $610/377$, and $1597/987$ we find a deviation for $L_0=L_0(\alpha)$ smaller than 10^{-5}.

B. Order parameter

Now, let us analyze the breakdown of analyticity near to the threshold ϵ_c in analogy to a phase transition of the second order. The first step towards a quantitative theory of continuous phase transitions is to identify an order parameter by which the phases involved in the phase transition are distinguished. Whereas the order parameter is zero in the disordered phase, it is nonzero in the ordered phase. With regards to the breakdown of analyticity, the nonzero order parameter appears in the discrete phase, which measures the discrete jumps in the hull functions. Our numerical results offer that the breakdown of analyticity can be completely discussed in terms of the hull function, instead of calculating the gap in the phonon spectrum as done in [30]. In the case $\epsilon<\epsilon_c$ the order parameter is zero whereas it is nonzero above ϵ_c. Here, we use the definition

$$\Phi = \frac{\int_0^1 \left| \frac{\partial f(z)}{\partial z} \right|^2 dz}{\delta(0)}, \tag{20}$$

where $f(z)$ can be identified with one of the different hull functions. The denominator is meant symbolically as a continuous limit. The calculations are performed in a discrete version with a finite number of particles. In that case $\delta(0)$ behaves like $\delta(0) \sim (\Delta z)^{-1} \equiv N_a$. If the hull function is

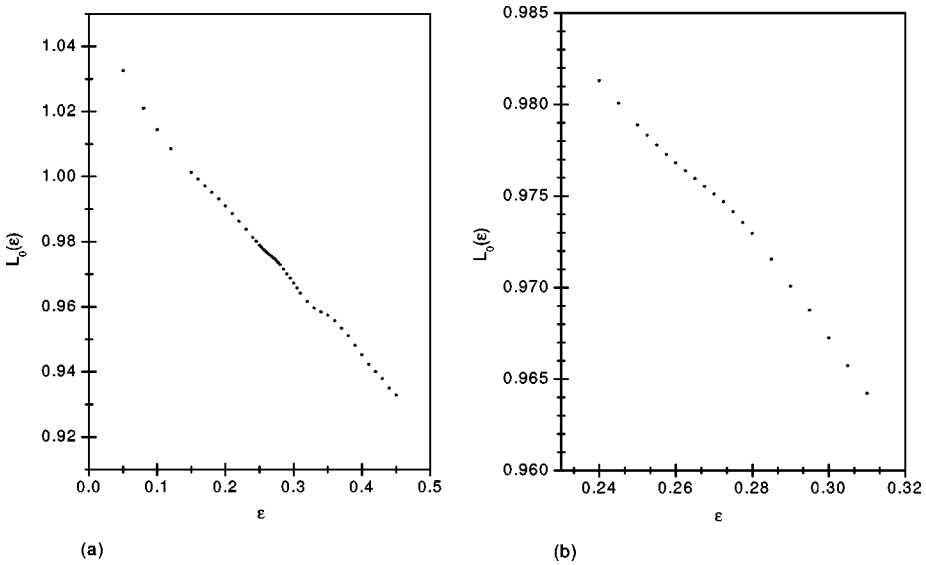

FIG. 5. The mean interaction distance L_0 in the y direction between the upper and lower chains as a function of interaction strength ϵ. The mean distance L_0 is plotted in different ranges (a) from $\epsilon=0.05,\ldots,0.4$ and (b) from $\epsilon=0.24,\ldots,0.31$ (transition range).

smooth within the interval $[0,1]$, the integral becomes finite and the order parameter vanished due to the prefactor $\delta(0)^{-1}$. On the other hand, if $f(z)$ behaves like a Heaviside function with a jump at z_0, we obtain $\partial_z f(z)\sim\delta(z-z_0)$ and therefore $\int_0^1[\partial_z f(z)]^2dz\sim\int_0^1\delta(z-z_0)^2dz\sim\delta(0)\int_0^1\delta(z-z_0)\sim\delta(0)$; i.e., the order parameter becomes finite. Due to the finite system size, which divides the region of integration into equidistant subintervals $\Delta z=1/N_a$ ($\Delta z=1/N_b$) for the upper (lower) chain, the integral in Eq. (20) is reduced to a sum over the particle numbers. Therefore, we have intrinsic discontinuities in the numerical computation, because the hull functions are given by a discrete set of points. In order to suppress the effects of these intrinsic discontinuities, we choose for the numerical investigation the generalized order parameter likewise denoted as Φ:

$$\Phi=\frac{\int_0^1\left|\frac{\partial^4 f(z)}{\partial z^4}\right|^2dz}{\delta(0)}\equiv\frac{1}{(\Delta z)^6}\sum_{k=2}^{\substack{(N_b-2)\\ N_a-2}}(|f_{k+2}-4\,f_{k+1}+6\,f_k-4f_{k-1}+f_{k-2}|)^2. \tag{21}$$

It should be mentioned that the order parameter Φ shows for all hull functions $f=\{h_a,h_b,h_c,h_d\}$ the same qualitative behavior. Therefore, in order to present the basic features of the phase transition (transition of the breakdown of analyticity) it is enough to calculate Φ [via Eq. (21)] for one hull function—e.g., $h_a=h_a(z)$.

C. Scaling behavior

In this subsection we present the order parameter Φ, defined by Eq. (21), for different system sizes $\alpha_n=89/55$, 233/377, 610/377, and 1597/987. Figure 6 shows the order parameter as a function of the interaction strength ϵ in the transition region. The results indicate clearly that the order parameter Φ changes from zero below the critical threshold ϵ_c to a nonzero value above ϵ_c for all particle number ratios. This is clear evidence for a phase transition of the second order. Using finite-size scaling arguments [37,38] for the data, presented in Fig. 6, the order parameter can be rewritten as

$$\Phi(\epsilon,L)=L^{\beta/\delta}\tilde{\Phi}(L^{1/\delta}(\epsilon-\epsilon_c)). \tag{22}$$

Below ϵ_c there is no static friction. This result is in accordance with [20–22] obtained by a completely different approach. Analyzing the data for different values of the system

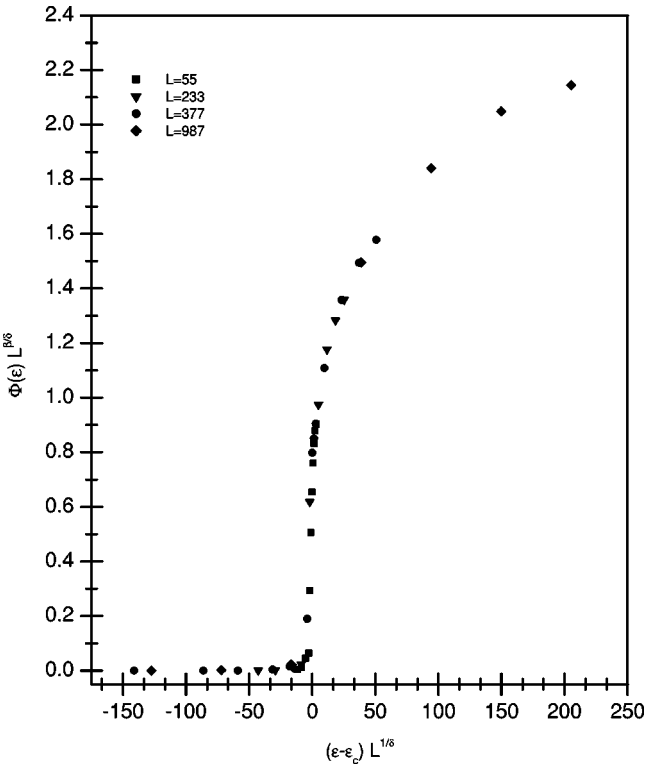

FIG. 6. Order parameter $\Phi(\epsilon)L^{\beta/\delta}$ versus $(\epsilon-\epsilon_c)L^{1/\delta}$.

size L (compare Fig. 6), we find that the order parameter offers a scaling behavior in the vicinity of the transition regime. That means that all curves for different L offer a data collapse. The corresponding master curve is depicted in Fig. 6. The system size L is determined by the particle numbers 55, 233, 377, and 987. In the transition region, characterized by the reduced interaction strength $t=(\epsilon-\epsilon_c)/\epsilon_c$, we find that the data of Fig. 6 are consistent with the following scaling behavior for $\epsilon>\epsilon_c$:

$$\Phi(\epsilon) \sim L^{\beta/\delta}(\epsilon-\epsilon_c)^{\beta}, \tag{23}$$

where the critical exponents are given by $\beta=0.239\pm0.05$ and $\delta=0.687\pm0.05$. From this we conclude the ratio $\mu=\beta/\delta \approx 0.347\pm0.05$. Due to the finite-size scaling, we obtain for the threshold interaction strength of the transition of breaking of analyticity the critical value $\epsilon_c=0.25575\pm0.001$.

IV. CONCLUSIONS

We have investigated the ground state for a two-dimensional double-chain model with an incommensurate lattice structure. We found that the structure of the hull functions depends strongly on the strength ϵ of the interaction between the upper and lower bodies. The breakdown of analyticity in the ground state for the critical value $\epsilon_c=0.25575$ was numerically observed. Furthermore, it was shown that this type of phase transition could be uniformly described by an order parameter. This order parameter representation allows a systematic analysis of the critical behavior for $\epsilon>\epsilon_c$ due to the calculation of the critical exponents. Consequently, the peculiar breakdown of analyticity shows all features of a second-order phase transition. As pointed out in the Introduction, the breaking of analyticity (Aubry transition) offers a transition from an unpinned to a pinned state. On the other hand, the relation between sufficiently small mean velocities and the external forces can be written as [27]

$$\overline{v} \propto (F-F_t)^{\zeta}, \tag{24}$$

where ζ is a universal exponent and F_t is the threshold force. In the unpinned state ($\epsilon<\epsilon_c$) a ground state can be continuously transformed into another ground state without any expenditure of energy. Thus the threshold force F_t is zero for $\epsilon<\epsilon_c$. For $\epsilon>\epsilon_c$ the broken analyticity prevents a smooth evolution between arbitrary ground states; i.e., we expect a finite threshold F_t for this regime.

Furthermore, it should be remarked that our chain model is a simple model structure, which established the macroscopic dry friction situation on the microscopic level between atomically flat surfaces by using a simply driven mechanical many-body system. It is convenient to define the model as simply as possible in order to discuss some basic features like the ground-state structure or the maximum static friction behavior. The validity of the underlying model system is given by the assumption of simple harmonic intrachain and Lennard-Jones interchain interactions. Referring to the comparison with experiments, another natural extension of the present model is to proceed to a three-dimensional system, which is able to describe wearless dry friction between two atomically flat planes pinned in each case to a substrate and embedding in a three-dimensional space.

We have only analyzed the situation for a fixed set of elastic parameters k_I. In further papers we will investigate this model for a wide range of the parameter set—e.g., the variation of the rigidity of one chain ($k_b=1,\ldots,\infty$).

ACKNOWLEDGMENTS

This work has been supported by the Graduiertenkolleg "Defektstrukturbestimmte physikalische Eigenschaften" and by the Deutsche Forschungsgemeinschaft DFG (Grant No. SFB 418).

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