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Emergent friction in two-dimensional Frenkel-Kontorova modelsJesper Norell,^{1,*} Annalisa Fasolino,² and Astrid S. de Wijn^{3,1,†}¹*Department of Physics, Stockholm University, 106 91 Stockholm, Sweden*²*Radboud University, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands*³*Department of Engineering Design and Materials, Norwegian University of Science and Technology, Trondheim, Norway*

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Simple models for friction are typically one-dimensional, but real interfaces are two-dimensional. We investigate the effects of the second dimension on static and dynamic friction by using the Frenkel-Kontorova (FK) model. We study the two most straightforward extensions of the FK model to two dimensions and simulate both the static and dynamic properties. We show that the behavior of the static friction is robust and remains similar in two dimensions for physically reasonable parameter values. The dynamic friction, however, is strongly influenced by the second dimension and the accompanying additional dynamics and parameters introduced into the models. We discuss our results in terms of the thermal equilibration and phonon dispersion relations of the lattices, establishing a physically realistic and suitable two-dimensional extension of the FK model. We find that the presence of additional dissipation channels can increase the friction and produces significantly different temperature dependence when compared to the one-dimensional case. We also briefly study the anisotropy of the dynamic friction and show highly nontrivial effects, including that the friction anisotropy can lead to motion in different directions depending on the value of the initial velocity.

DOI: [10.1103/PhysRevE.94.023001](https://doi.org/10.1103/PhysRevE.94.023001)**I. INTRODUCTION**

Friction between sliding surfaces is a common phenomenon which plays an important role in everyday life. Like all transport properties, however, friction is ultimately the result of microscopic interactions between particles. Recent years have witnessed a surge of interest in understanding the microscopic origin of friction, due to the increased control in surface preparation and the development of nanoscale experimental methods such as Quartz Crystal Microbalance [1] and Friction Force Microscopy [2]. A considerable amount of this effort is being directed towards reducing friction. One way to reduce friction is through incommensurability, i.e., structural incompatibility between the sliding surfaces on the atomic level. This effect, often called structural superlubricity [3–5], has been observed experimentally in nanoscale contacts, for example in graphite [6].

Theoretical studies of incommensurate sliding contacts often employ the Frenkel-Kontorova (FK) model [3,7–9] or extensions (see, for example, Ref. [10]). Crucially, the FK model does not assume that the sliding objects are rigid. This allows it to describe deformations of the lattice, which can destroy the vanishing static friction [5] for sufficiently soft materials. The FK model can also describe phonons and heat in the lattices, which absorb the kinetic energy of the sliding [4]. Consequently, the FK model is the simplest model in which dynamic friction is emergent, while in other models some form of heuristic damping must be included.

While the FK model has been studied extensively in one dimension, its two-dimensional (2D) extensions have not received as much attention. In two dimensions, both halves of the contact have at least two independent parameters describing the lattice, which considerably complicates the

concept of commensurability (see, for instance, Refs. [11,12]). Two-dimensional surfaces also have 2D phonon dispersion and at least two independent elastic constants. Recently there have been a number of studies dealing with the FK model in two dimensions that use several different 2D extensions. Several works (see, for example, Refs. [13,14]) consider a scalar harmonic interaction, which we will see here can cause serious problems with the dynamic friction. Other works use 2D springs for the interaction, but include only interactions between nearest neighbors (see, for example, Ref. [15]). For square lattices, this gives rise to an unphysically vanishing shear modulus and, as we will see here, unphysical friction. Another group that has mostly investigated scalar harmonic FK models [14] later also considered 2D next-nearest neighbor interactions [16], but, opposite to what one would expect, did not find any contribution to the dynamic friction from the dynamics inside the chain. Static friction of 2D sheets of colloids has also been studied in, e.g., models consisting of particles interacting with a Yukawa potential [17] instead of FK models. To the best of our knowledge, the impact of the functional forms of the different FK models in two dimensions and the values of their parameters on the static and dynamic friction have not yet been systematically compared and evaluated.

Here we investigate the impact of the second dimension on the frictional properties in the FK model. We consider the two most straightforward extensions to two dimensions and determine what is needed for describing the friction in a physical way, in both the static and dynamic case. We demonstrate how the second dimension affects the static and dynamic friction, and obtain several qualitatively new effects in terms of the temperature dependence of the friction coefficient and nontrivial anisotropy.

The paper is organized as follows. Section II introduces the basic features of the FK model, along with definitions and motivations of the 2D models and their parameters. Section III describes the static frictional properties. In Sec. IV we

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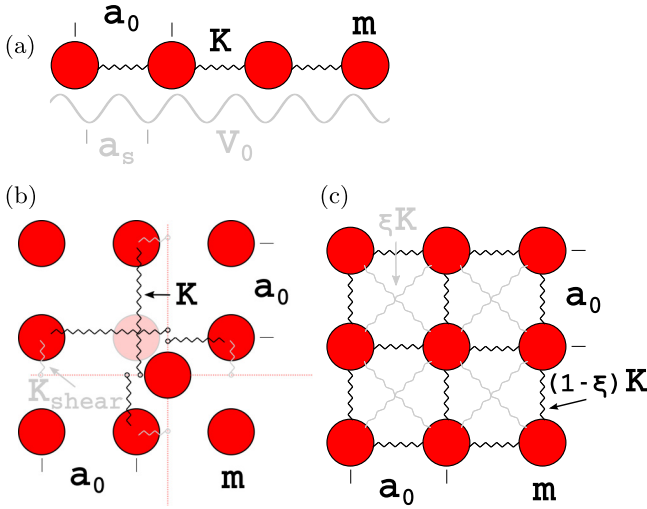


FIG. 1. Schematic illustrations of the 1D FK model (a) and the internal interaction of the two 2D extensions studied in this work, the scalar model (b) and vector model (c). In (b) the interaction is displayed only for the particle which has been distorted from the shaded equilibrium position, as the shear interaction equilibrium distance is zero.

investigate thermal equilibration within the models, in relation to sliding friction. Section V deals with the dynamic friction and the resulting effective viscous friction. The results are then interpreted in terms of the phonon dispersion relations of the lattices in Sec. VI. In Sec. VII we show several new effects that occur in two dimensions. Last, our conclusions are summarized in Sec. VIII.

II. MODELS

We first briefly discuss the one-dimensional (1D) FK model [7], which has been studied extensively [9]. It consists of N particles of mass m in an ordered harmonic chain with equilibrium spacing a_0 and spring constant K . The particles interact also with an external sinusoidal substrate potential of periodicity a_s and amplitude $V_0/2\pi$. The basic setup is shown in Fig. 1(a). Often the effects of inertia are neglected, and this is referred to as the static FK model. Inclusion of kinetic energy instead results in what is known as the dynamic FK model.

The commensurability of the system is characterized by the winding number w , the ratio of the mean interatomic distance and the period of the potential. A rational (irrational) value of w defines a commensurate (incommensurate) structure. As discussed in Sec. II D, for computational reasons, we use periodic boundary conditions that fix the mean interatomic distance at the unstretched length of the spring. Therefore w becomes equivalent to the ratio of the two length scales $r = a_0/a_s$. We focus only on the incommensurate case, which is both more likely for arbitrary surfaces in contact and more interesting in the context of structural lubricity.

The coupling parameter $\lambda = V_0/(Ka_s^2)$ describes the relative strength of the two interaction types. When λ is below a critical value λ_c (which depends on r) the incommensurate 1D FK model is in a floating state with zero static friction. For values $\lambda \geq \lambda_c$, however, the system enters a pinned state with finite static friction. This transition by breaking of analyticity is

known as the Aubry transition [5,18]. The parameter can in real systems vary strongly, but we focus here in particular on a value below the transition. The experimentally observed vanishing static friction of graphene flakes on graphite [6] strongly suggests that covalently bonded materials physisorbed on substrates are in this regime.

We use $r = \tau_g = (1 + \sqrt{5})/2$, i.e., the golden mean (which is the optimally incommensurate ratio [19]) $\lambda = 0.05 \approx \lambda_c/3$ [20], and employ the reduced units $m = 1$, $K = 1$, and $a_s = 1$, which yields the units of time $\tau_0 = \sqrt{m/K} = 1$ and energy $Ka_s^2 = 1$.

In the dynamic 1D FK model, an effective friction arises as a result of the Hamiltonian dynamics [4,21], as primarily caused by resonances between the sliding induced vibrations and phonon modes in the chain. For a uniform sliding of all the particles with velocity v^+ over the potential, a vibration with the washboard frequency $\Omega = 2\pi v^+/a_s$ is induced. The periodicity of the potential corresponds to a wave number of $q = 2\pi r$ for phonons in the chain. Resonances will therefore occur when the washboard frequency matches the phonon dispersion relation of the lattice $\omega = 2|\sin(k/2)|$ for $k = q$ or its harmonics nq , i.e., for the velocities

$$\tilde{v}_n^+ \sim \sin(n\pi r)/n\pi, \quad (1)$$

where $n = 1, 2, 3, \dots$ is the order of the resonance.

When the chain slides with a velocity at or near a resonance, the washboard frequency can parametrically excite acoustic phonon modes. The energy will then dissipate from these modes into other phonon modes [4], leading to friction and ultimately thermal equilibrium [21]. At zero temperature, this will be preceded by an initial recurrence [4,21], whereby a fraction of the total energy is transformed back and forth between internal degrees of freedom and the center of mass (CM) translation. At nonzero temperature, the thermal fluctuations speed up the decay, which becomes viscous from the beginning. The effective friction coefficient, however, depends on the velocity nontrivially, due to the interplay of resonances and thermal fluctuations.

A. Two-dimensional models

For the 2D models we consider the simplest possible lattice, namely, a square symmetry for both the elastic material and the substrate potential. This gives the straightforward generalizations of the Hamiltonian

$$\mathcal{H} = \sum_{j=1}^{N_x} \sum_{l=1}^{N_y} \left[\frac{|\dot{\vec{r}}_{j,l}|^2}{2} + V_{\text{ext}} + V_{\text{int}} \right], \quad (2)$$

$$V_{\text{ext}} = \frac{\lambda}{2\pi} [\cos(2\pi x_{j,l}) + \cos(2\pi y_{j,l})], \quad (3)$$

where $\vec{r}_{j,l} = (x_{j,l}, y_{j,l})$ is the position of particle (j, l) and $\dot{\vec{r}}_{j,l}$ the corresponding velocity. The internal potential energy of the sheet of particles is given by V_{int} . We also define the CM velocity as

$$\vec{v} = (v_x, v_y) = \frac{1}{N_x N_y} \sum_{j=1}^{N_x} \sum_{l=1}^{N_y} \dot{\vec{r}}_{j,l}. \quad (4)$$

The variables $\vec{r}_{j,l} = (x_{j,l}, y_{j,l})$ describe the microscopic internal degrees of freedom, while $\vec{v} = (v_x, v_y)$ is reserved for the macroscopic sliding.

Several different options have been previously considered for V_{int} , e.g., simple harmonic types [9,13,14] and multidimensional springs [9,15,16,22]. We evaluate these alternatives by considering two representative but qualitatively different interaction types, hereafter dubbed the scalar and vector model, which are schematically illustrated in Figs. 1(b) and 1(c).

The scalar model describes the two coordinate components as independent scalars with interaction energy terms for each particle j,l

$$V_{\text{scalar}} = \frac{K}{2}[(x_{j,l+1} - x_{j,l} - a_0)^2 + (y_{j,l+1} - y_{j,l} - a_0)^2] + \frac{K_{\text{shear}}}{2}[(x_{j,l+1} - x_{j,l})^2 + (y_{j,l+1} - y_{j,l})^2], \quad (5)$$

where K_{shear} measures the restoring force for transverse displacements within a subchain.

Importantly, for the scalar model the x and y coordinates of the particles decouple completely. As will be seen later, this has undesirable consequences for the dynamics and can lead to unphysical behavior.

The vector model conversely describes the vector nature of the particle displacements via fully 2D springs. We include the interaction between second nearest neighbors as described here by the internal interaction

$$V_{\text{vector}} = (1 - \xi) \frac{K}{2} [(|\vec{r}_{j+1,l} - \vec{r}_{j,l}| - a_0)^2 + (|\vec{r}_{j,l+1} - \vec{r}_{j,l}| - a_0)^2] + \xi \frac{K}{2} [(|\vec{r}_{j+1,l+1} - \vec{r}_{j,l}| - \sqrt{2}a_0)^2 + (|\vec{r}_{j+1,l-1} - \vec{r}_{j,l}| - \sqrt{2}a_0)^2], \quad (6)$$

where $0 \leq \xi \leq 1$ controls the relative strength of the two interactions.

B. Model parameters

To understand the meaning of the two new model parameters, it is instructive to consider the effective elastic constants c_{11} (longitudinal stretching) and c_{44} (transverse shearing) of the lattices. For the scalar case one obtains trivially $c_{11}/c_{44} = K/K_{\text{shear}}$, whereas Taylor expansion to first order of the vector model yields $c_{11}/c_{44} = K/\xi K$. The 2D elastic properties of the models are therefore expected to be most alike if the ratios are equated:

$$K_{\text{shear}} = \xi K. \quad (7)$$

Both models preserve the elastic properties of the 1D model in their longitudinal stretching, while the shearing can be tuned independently. The latter point has particular consequences for the vector model: the case $\xi = 0$ yields a zero shear modulus with strong effects on the friction as shown later, whereas $\xi = 1$ results in a model of two such intertwined but independent lattices.

To estimate realistic values for the two parameters one can consider, for example, the properties of solidified rare gases often employed as the elastic material in Quartz Crystal Microbalance studies of friction [23], e.g., xenon [24], $c_{11}/c_{44} = 2.01$, and krypton [25], $c_{11}/c_{44} = 2.08$, i.e., $c_{11}/c_{44} \approx 2$. However, since such measurements are performed on three-

dimensional (3D) crystals one needs in the vector model to account for the higher number of next-nearest neighbors in three dimensions. The correct expression for comparison therefore becomes $c_{11}/c_{44} = (1 + \xi)K/2\xi K$, which gives $K_{\text{shear}} \approx 0.5$ and $\xi \approx 0.33$ as our estimation of representative values.

C. Lattice phonon dispersion

The friction of the 1D FK model, and the associated resonances in particular, depends strongly on the phonon dispersion relation of the elastic lattice.

The phonon dispersion in one dimension, calculated in textbook examples [26], is readily extended to the scalar model due to the decoupled equations of motion. One obtains

$$\omega = \pm 2 \left[K \sin^2 \left(\frac{k_x a_0}{2} \right) + K_{\text{shear}} \sin^2 \left(\frac{k_y a_0}{2} \right) \right]^{1/2} \quad (8)$$

for x polarization, and equivalently for y polarization with $x \rightleftharpoons y$.

The two branches are shown as curves between important points in the first Brillouin zone (FBZ) in Fig. 2(a). The x polarized branch is additionally shown for the entire FBZ in Fig. 2(b) and 2(c) for $K_{\text{shear}} = 0.5$ and 1.

For the vector model we apply the harmonic approximation, which together with the Ansatz function

$$\vec{z}_{j,l}(t) = \begin{bmatrix} \Delta x(k_x, k_y) \\ \Delta y(k_x, k_y) \end{bmatrix} e^{i(\omega t + k_x j a_0 + k_y l a_0)} \quad (9)$$

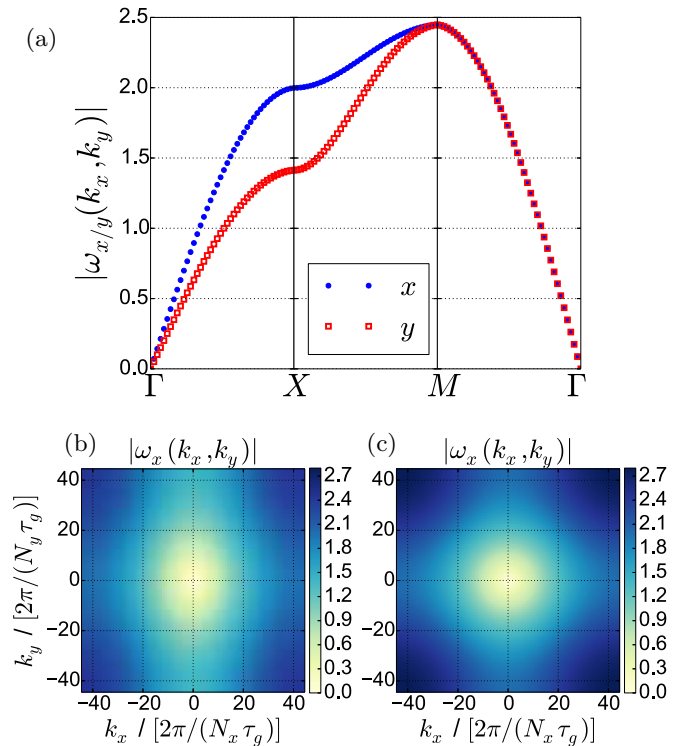


FIG. 2. Phonon dispersion for the scalar model: for $K_{\text{shear}} = 0.5K$ between the three points $\Gamma = (0,0)$, $X = (\pi,0)$, $M = (\pi,\pi)$ for the x (blue points) and y (red squares) polarized branches (a), and 2D phonon dispersion maps of the x polarized branch for $K_{\text{shear}} = 0.5$ (b) and 1 (c).

gives the equations of motion

$$-\frac{d^2}{dt^2} \vec{z}_{j,l} = \underline{D}(k_x, k_y) \vec{z}_{j,l} = \omega^2 \vec{z}_{j,l} \quad (10)$$

with the symmetric dynamical matrix

$$\underline{D} = \frac{4K}{m} (1 - \xi) \underline{D}^\alpha + \frac{2K}{m} \xi \underline{D}^\beta, \quad (11)$$

$$\underline{D}_{1,1}^\alpha = \underline{D}_{2,2}^\alpha = \sin^2(k_x a_0 / 2), \quad (12)$$

$$\underline{D}_{1,2}^\alpha = \underline{D}_{2,1}^\alpha = 0, \quad (13)$$

$$\underline{D}_{1,1}^\beta = \underline{D}_{2,2}^\beta = [1 - \cos(k_x a_0) \cos(k_y a_0)], \quad (14)$$

$$\underline{D}_{1,2}^\beta = \underline{D}_{2,1}^\beta = \sin(k_x a_0) \sin(k_y a_0). \quad (15)$$

Diagonalization of the dynamical matrix yields the phonon dispersion shown in Fig. 3 for $\xi = 0.33$. Results for the entire FBZ are shown in Figs. 3(b) and 3(c).

For $\xi = 0$, the 1D phonon dispersion is recovered. However, the harmonic approximation for $\xi = 0$ for the transverse modes yields vanishing coefficients and a phonon dispersion relation with $\omega = 0$ for all wave vectors. These zero frequency vibrational modes do not occur in physical systems, and, as we will see later, for a reasonable description of the dynamic friction it is crucial to exclude them from the model.

D. Computational details

We integrate numerically the equations of motion with a fourth order Runge-Kutta algorithm. The time step of $\tau_0/150$

preserves the total energy to at least three digits over the duration of our runs. As we simulate a finite-size system, with periodic boundary conditions [i.e. $\vec{r}_{j,l} = \vec{r}_{j \pm N_x, l} \mp (N_x a_0, 0) = \vec{r}_{j, l \pm N_y} \mp (0, N_y a_0)$], we must approximate the ratio of lattice parameters by a nearly incommensurate rational ratio

$$r = \frac{F_{n+1}}{F_n} \approx \tau_g, \quad (16)$$

where F_n is the n th Fibonacci number. Unless mentioned explicitly we choose as the system size $N_x = N_y = 89$ and thus $a_0 = 144/89$. We restrict ourselves to the case of lattice vectors aligned with the substrate potential.

To obtain initial conditions at a specific temperature (0 for energy minimization), we first place the particles in the equidistant equilibrium configuration of the elastic square lattice. Then we apply a Langevin thermostat with damping parameter 0.5 for 10^5 time steps, after which the thermostat is removed. We note that the minimization procedure does not necessarily give the true ground state (GS), i.e., the global energy minimum, of the models. However, for the sake of comparing the qualitative static properties of the 2D models, we consider the numerical approach sufficient.

To study the Hamiltonian dynamics of the system we follow the procedure of Ref. [21]. At $t = 0$, we give every particle an equal velocity increment v_x^+ in the x direction, so that the sheet of particles starts sliding on the substrate. After this the Hamiltonian dynamics are monitored without further interference.

III. STATIC FRICTION

Before investigating the dynamics of the 2D extensions of the FK model, we first discuss the static friction and the GS. The GS can be described in terms of the modulation function f and hull function g , respectively [5]:

$$f(i a_0 \bmod a_s) = u_i \bmod a_s, \quad (17)$$

$$g(i a_0 \bmod a_s) = u_i - i a_0, \quad (18)$$

where the transition from zero to finite static friction (the Aubry transition) can be identified by the emergence of discontinuities in f (or equivalently g). We calculate numerically the modulation function by using the displacements with respect to constant spacing of the ground state obtained from energy minimization. This procedure gives an approximation of the exact continuous or discontinuous function by a discrete set of points.

For the scalar model, the GS configuration can be found directly from the GS of the 1D FK model. Let us denote the position of a particle i in the GS of the 1D model as q_i . We find by direct insertion that the configuration

$$(x_{j,l}, y_{j,l})_{\text{GS}} = (q_j, q_l) \quad (19)$$

fulfills the GS criterion of zero force, independently of K_{shear} . The particles line up within x and y subchains in the positions of the 1D GS, which leaves the static friction unaffected by the extensions.

For the vector model, Eq. (19) gives only the exact GS in the limiting case of $\xi = 0$. When $\xi > 0$, the interaction between next-nearest neighbors distorts the GS. However, we find that the distortion is typically weak in the interesting parameter

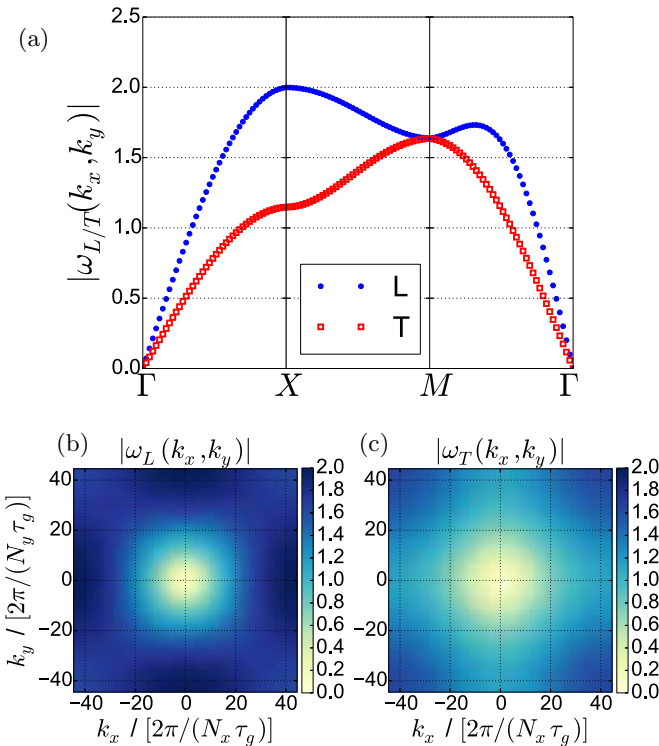


FIG. 3. Phonon dispersion for the vector model: for $\xi = 0.33$ between the three points $\Gamma = (0,0)$, $X = (\pi,0)$, $M = (\pi,\pi)$ for the longitudinal (L, blue points) and transverse (T, red squares) branches (a), and 2D phonon dispersion maps for $\xi = 0.33$ of the (quasi-)longitudinal modes (b) and (quasi-)transverse modes (c).

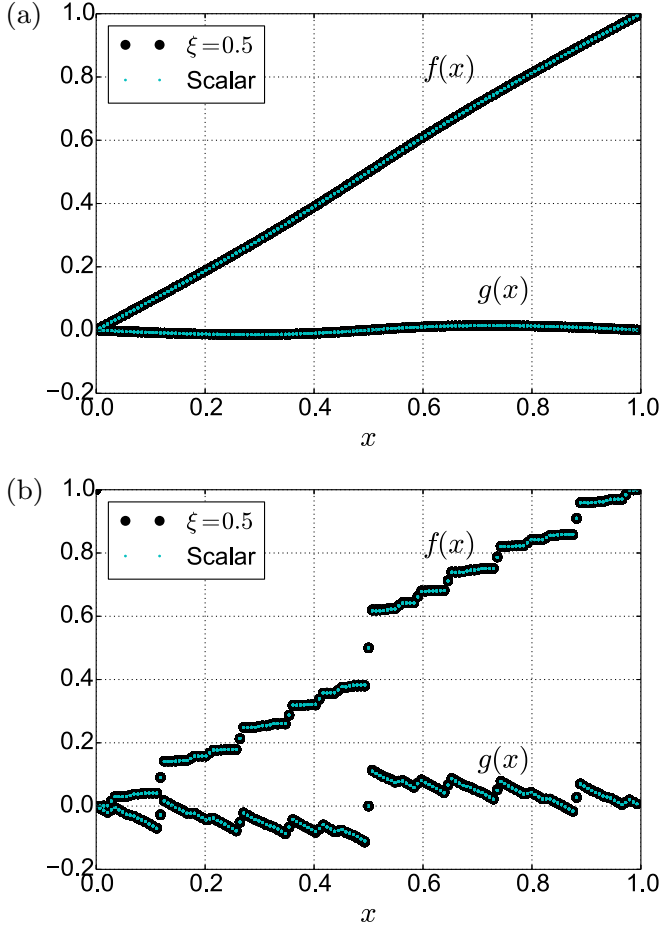


FIG. 4. Numerically obtained modulation $f(x)$ and hull $g(x)$ functions of the x subchains (particles with identical l) in the vector model (with $\xi = 0.5$, large black dots) and the scalar model (small cyan dots) for (a) $\lambda = 0.05$, a floating state below the Aubry transition and (b) $\lambda = 0.20$, a pinned state above the Aubry transition. The results are nearly identical for the two models. Results with equivalent similarities between the models have also been obtained for several values $0 \leq \lambda \leq 0.25$, while a further increase of ξ leads eventually to an appreciable alteration of the functions.

ranges. This can be seen in Fig. 4, which shows results obtained by numerical energy minimization for the vector model with $\xi = 0.5$ as compared to the scalar model [32]. The results are nearly identical for the two models both above and below the Aubry transition.

We thus conclude that in the physically relevant parameter range the different models describe the Aubry transition and the static friction in a very similar way, that is, also similar (or even identical) to the 1D case. All cases considered in the following sections, i.e., $\lambda = 0.05 \approx \lambda_c/3$ and $\xi \leq 0.5$, are thereby approximately equivalent to the 1D case in terms of static properties.

IV. EQUILIBRATION

To investigate the dynamic friction, we add a velocity v_x^+ to the CM and monitor the decay to equilibrium. The dissipation of CM motion into internal energy (phonons) and subsequent decay are key features of the FK model. However, there are

many ways in which the equilibration can be slowed down or inhibited, e.g., if the systems are too small [3,4]. Here we therefore first examine if the different extensions of the FK model to two dimensions correctly describe the process of thermal equilibration.

A. Harmonic equipartition

In thermal equilibrium the systems should obey equipartition. For (approximately) harmonic interaction, this means that the energy should be divided on average equally between kinetic energy E_k and relative potential energy $E_p - E_0$. To determine if equipartition is obeyed, we monitor these energies as a function of time after the initial CM velocity increase.

Typical cases are shown in Figs. 5(a) and 5(d). As these systems were started from zero temperature, one observes an initial recurrence, followed by an approximately exponential decay of the CM velocity, after which it starts to jiggle thermally around a zero mean.

We see that the expected equipartition is reached for both the scalar model and the vector model for sufficiently large values of ξ . For the vector model with small values of ξ (not shown), however, the harmonic approximation is no longer valid at the energies in our simulations, and thus harmonic equipartition is neither expected nor obeyed.

B. Thermal distributions

As a second test, we check if the CM velocity obeys the Maxwell-Boltzmann (MB) distribution.

For the scalar model, we find that the x component of the CM velocity obeys a MB distribution, but the y component does not, as can be seen in Figs. 5(b) and 5(c). This exposes clearly the previously mentioned flaw of the model: the scalar nature of the internal interaction causes a complete decoupling in the equations of motion between the x and y components, resulting effectively in two independent 1D models. There is therefore no equilibration between the different components, and the kinetic energy from a velocity increment in the x direction never dissipates into vibrations in the y direction. Moreover, because these simulations start from the ground state, each independent subchain has the same initial conditions. Therefore, the energy is redistributed only over N_x independent degrees of freedom, not $2N_x N_y$. As a result, the temperature of the MB distribution is approximately a factor of $2N_y$ too high. While the symmetry between the subchains can be broken by initial conditions, such as an initial temperature, the decoupling between x and y is inherent in the dynamics. For this reason, the scalar model is clearly not suitable as a fully 2D extension for the dynamic FK model.

The vector model, conversely, is well behaved for physical parameter values ($0.01 \leq \xi \leq 0.5$). For both x and y components the CM velocity obeys the MB distribution corresponding to the correct temperature. Only for $\xi = 0$ with zero temperature the system does not equilibrate properly. This is due to the symmetry of the initial conditions, which is preserved by the symmetry of the dynamics. As a result, the nonlinear terms never become relevant. At finite temperature, this symmetry is broken and equilibration is restored.

In many cases for the vector model, however, we find that while the temperatures do converge, this convergence is very

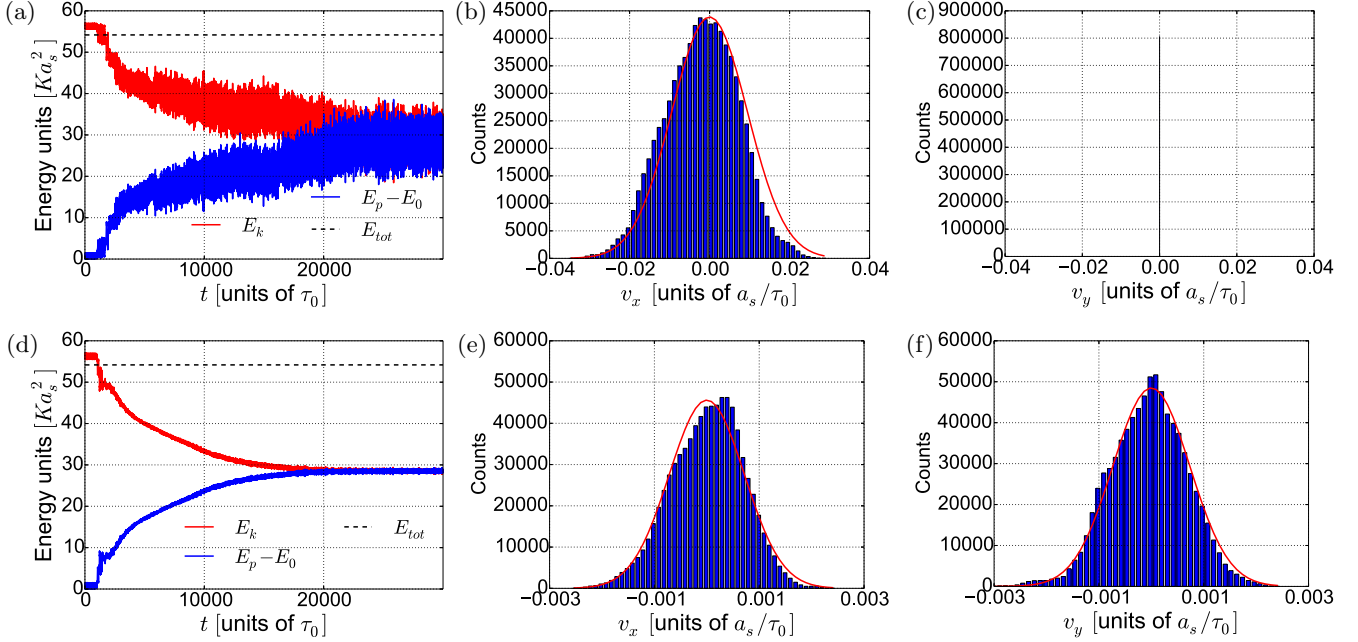


FIG. 5. Indicators of thermal equilibration, for the scalar model with $K_{\text{shear}} = 0$ and 1 (the results are independent of the K_{shear} value) (top) and for the vector model with $\xi = 0.33$ (bottom). Subfigures (a) and (d) show the time evolution of the kinetic (red upper solid line), potential (blue lower solid line), and total (black dashed line) energies, after a CM velocity increase of $v_x^+ = 0.12$ (a resonant value) from the GS. The energies clearly display equipartition, after the initial recurrence. The histograms of the CM velocity components for x and y components are for the scalar model in (b) and (c) and for the vector model in (e) and (f) with fitted Gaussian functions (red lines). The histograms were obtained by binning the velocity components over a time period of $9 \times 10^5 \tau_0$, starting after an initial equilibration time of $10^5 \tau_0$. Results for almost all other parameter values are comparable. For small ξ equipartition is neither expected nor observed and for $\xi = 0$ due to symmetry equilibration fails.

slow. In order to obtain enough statistics and satisfactorily confirm equilibration, we were sometimes forced to resort to computationally cheaper smaller systems and simulate for much longer times. It thus appears that all the vector model systems (with $0 < \xi \leq 0.5$) do equilibrate eventually, but that the process can be very slow.

We also note that equilibration was obtained for the vector model with the surprisingly small size $N_x = N_y = 34$ (on 21 periods of the potential). For the scalar model and 1D FK, $N = 34$ is too small for dissipation: there is no decay of the velocity as the system never leaves the initial recurrence. Thus, we can also conclude that the nonlinear coupling in the vector model not only provides equilibration between x and y , but also helps equilibration in small systems.

We have not investigated the system-size dependence systematically, but note that in the vector model with our parameters, for $N_x = N_y = 13$ (on eight periods of the potential), the initial recurrence survives for an extremely long time ($\sim 200\,000 \tau_0$) even at resonant velocities. The authors of Ref. [16] investigate an even smaller system, $N_x = N_y = 12$; we suspect that this is why they did not observe any dissipation due to internal motion.

V. VISCOUS FRICTION

When a finite initial temperature is introduced in the system, the CM velocity decays more rapidly, as if subjected to an effective viscous friction. We can thus extract an effective viscous friction coefficient η by fitting of an exponential

function to the decay curve in a similar way as in the 1D case [21].

In the results presented below, we fit both the coefficient in the exponent and the prefactor of the exponential function to the average decay curve of at least 100 trajectories (300 for the 1D system) obtained from different initial conditions (generated by differently seeded thermostats). Once the CM velocity has decayed enough, the internal temperature of the sheet of particles increases. We therefore fit only to an initial period, where the temperature is relatively constant, in this case the first $1000 \tau_0$. An example of the ensemble average and the fit is shown in Fig. 6. In the following we consider the low-temperature case $T = 0.022\lambda$, which has shown clear resonance peaks in the 1D case [21].

In Sec. VA we first confirm that the resonance peaks in the friction that appear in the 1D systems survive in the extension to 2D. In Sec. VB we then investigate how the new parameters of the 2D models affect the friction. Explanations for the observed results are presented in Sec. VI.

A. Velocity dependence and resonances

In Fig. 7 we show how the friction coefficient depends on the velocity v_x for several values of K_{shear} in the scalar model (a) and ξ in the vector model (b), in comparison to the 1D results.

The scalar model is found to behave much like its 1D counterpart. In the limiting case $K_{\text{shear}} = 0$ the results are identical, as the system then reduces to $N_y = 89$ independent 1D chains. Results for larger $K_{\text{shear}} \leq 1$ remain comparable.

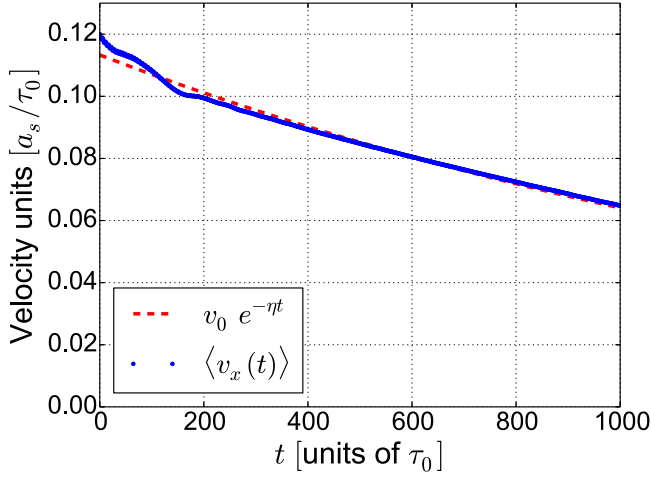


FIG. 6. The averaged CM velocity decay of the vector model (blue points) with $\xi = 0.33$, $v_x^+ = 0.12$, and initial temperature $T = 0.16\lambda$. The dashed red line shows the exponential fit in the range $0 \leq t \leq 1000\tau_0$ from which the effective viscous friction coefficient η is obtained.

The introduction of a shear interaction with a reasonable K_{shear} value has qualitatively two effects: an increase of friction for resonant velocities and a suppression of friction for nonresonant velocities. The increase is more pronounced for smaller values of K_{shear} , whereas the suppression appears with strong shear interaction.

For the vector model the velocity-dependence changes drastically with the model parameter ξ . For small values of $\xi \gg 0.01$ the friction is orders of magnitude higher than for larger values, as shown in the inset of the figure on a logarithmic scale. The friction also decreases with increased initial velocity. This result is pathological and related to the unrealistic, (nearly) vanishing c_{44} constant, yielding a transverse branch of phonon modes with extremely low frequency. Phonon modes with low or zero frequency can absorb energy easily, especially in combination with strong nonlinearity, and thus for small values of ξ , the modes involving transverse motion rapidly absorb energy and cause extremely high friction.

For $\xi = 0.1$, there is a qualitative agreement with the 1D and scalar models for low velocities. For high velocities, however, the friction increases dramatically and behaves similarly to the friction for smaller ξ . For the more reasonable $\xi = 0.33$, the agreement between the 1D and 2D cases extends to all the simulated velocities. As for the scalar model, we find in this case a larger friction at the resonances than in the 1D case.

Last, $\xi = 0.5$ results in a higher friction for low velocities and the apparent appearance of a third resonance peak. Following the procedure of Sec. VI, we find that the peak is not, unlike the other two, due to a resonance in the x subchains. Energy is instead absorbed in modes with a wave vector oriented along the lattice diagonal, as the next-nearest and nearest neighbor interaction is equally strong to first order for this parameter value. It is not clear to us whether there exists real materials where such an effect could be observed.

B. Model parameters

We now investigate in more detail the dependence of η on the two new parameters K_{shear} and ξ for both resonant and

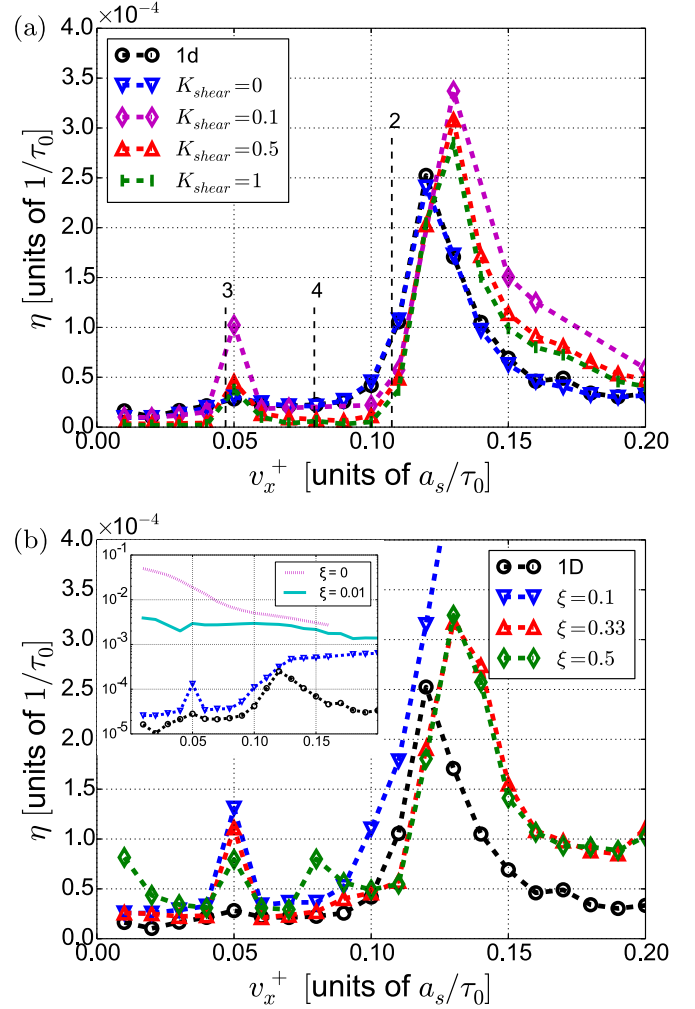


FIG. 7. The effective viscous friction as a function of initial velocity $\eta(v_x^+)$ for the scalar (a) and vector (b) models, compared to the 1D case, for initial temperature $T = 0.022\lambda$. Results for small values of ξ are shown in an inset with logarithmic scale. Red lines (with upwards pointing triangles) correspond to models with the ratio $c_{11}/c_{44} = 2$; other colors are not directly comparable between the figures. Resonances and their order (vertical dashed lines) apply in both cases, but have been omitted in the lower panel to not obscure the results.

nonresonant sliding velocities. Figure 8 shows the results for a wide range of values of the model parameters and for three different initial velocities: one resonant ($v_x^+ = 0.05$) and two nearby nonresonant ($v_x^+ = 0.03, 0.07$).

For the scalar model, shown in Fig. 8(a), we find a weak dependence for small values of $K_{\text{shear}} \lesssim 0.1$, and a monotonous decrease thereafter. Only for extremely unrealistic values $K_{\text{shear}} \gtrsim 10$ do the curves for the different velocities meet. The resonance is thus preserved throughout the range of reasonable K_{shear} .

The vector model, shown in Fig. 8(b), is qualitatively different. At low values of ξ , the friction coefficient is orders of magnitude higher than that of the scalar model, but also depends only weakly on ξ . At the intermediate values of ξ , the friction coefficient decreases and is similar to that of

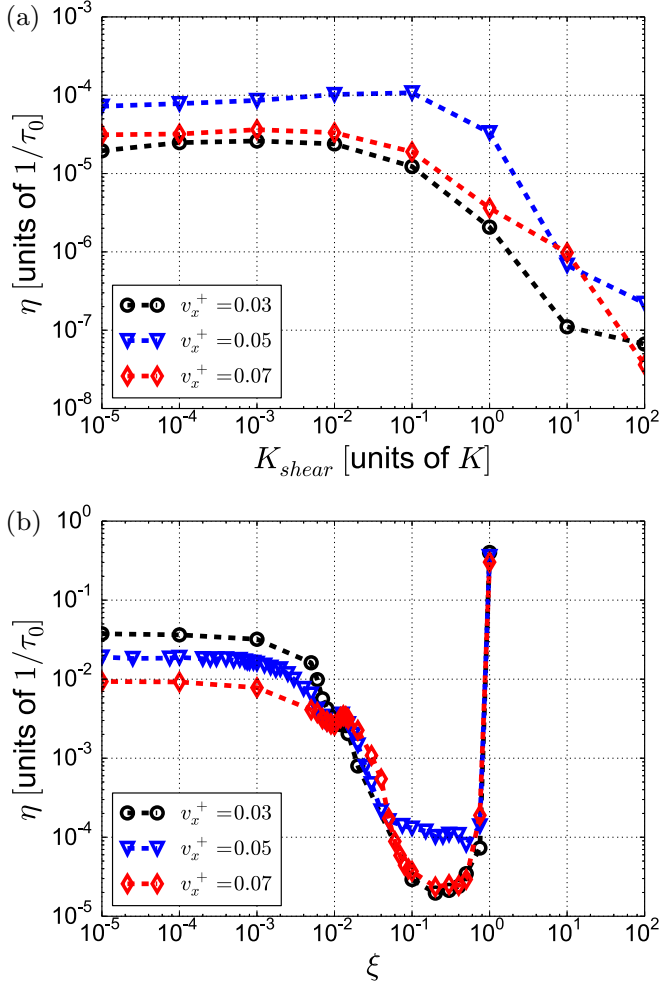


FIG. 8. The viscous friction η as a function of K_{shear} in the scalar model (a) and ξ in the vector model (b) for three different initial velocities and initial temperature $T = 0.022\lambda$. The values $v_x^+ = 0.03, 0.05, 0.07$ correspond to a resonant value (0.05) and two nearby nonresonant values. The elastic behavior of the models can be compared through the relation in Eq. (7).

the scalar model for equivalent K_{shear} parameters. Finally, for large values of $\xi \gtrsim 0.7$ up to the maximum of $\xi = 1$, the friction increases, as the system begins to separate into two independent lattices, consisting of the previously next-nearest neighbors, similar to the $\xi = 0$ case but with a less incommensurate lattice spacing.

It is thus only in the region of $0.1 \lesssim \xi \lesssim 0.7$, i.e., $1.22 \lesssim c_{11}/c_{44} \lesssim 5.5$, where the predicted resonance can be found. Interestingly, 74 out of 88 (84%) cubic single crystals found in Ref. [27] are also in this range. We therefore expect the resonance behavior to be the rule rather than the exception also in 2D systems.

VI. PHONON MODE POPULATIONS

To explain the trends observed in the last section, we now turn our attention to a direct connection between the sliding dynamics and the lattice phonon dispersion. Through the time development of the phonon mode populations we

determine how energy is transferred to vibrational modes and consequently dispersed in the vibrational spectrum, which gives detailed insight in the mechanism of dissipation. A discrete Fourier transform of the coordinates is performed as defined by [28]

$$A_{j,l}(x) = \sum_{s=0}^{N_x-1} \sum_{t=0}^{N_y-1} x_{s,t} e^{-i(s\Omega_j + t\Omega_l)}, \quad (20)$$

$$\Omega_j = 2\pi j/N_x; \quad j = 0, 1, \dots, N_x - 1, \quad (21)$$

$$\Omega_l = 2\pi l/N_y; \quad l = 0, 1, \dots, N_y - 1, \quad (22)$$

and equivalently for the $A_{j,l}(y)$ component with $x_{s,t} \rightarrow y_{s,t}$. The power $|A_{j,l}(w)|^2$ is then a direct indicator of the population in mode $(j,l) = (k_x, k_y)$ of polarization $w \in \{x, y\}$ in the scalar model. For the vector model this is not strictly the case, as the $x - y$ coupling in the interaction causes the modes to not be purely x or y polarized, except in specific symmetry directions. Nevertheless, we find that these coordinates are sufficient for a qualitative analysis.

Shown in Figs. 9 and 10 are the Fourier transformed coordinates for the scalar model with $K_{shear} = 0.5$ and vector model with $\xi = 0.33$ respectively, in the case of $T = 0.022\lambda$. We choose $v_x^+ = 0.12$ to illustrate resonant behavior. Results are shown for the time points $t = 0$ (just before the velocity increment), $t = 50\tau_0$ (showing the initial conversion of sliding energy), and $t = 1000\tau_0$ (illustrating a longer term redistribution of energy).

For $t = 0$ in both cases [Figs. 9(a), 9(b), 10(a), and 10(b)] we find a number of peaks in longitudinal modes with wave vectors corresponding to the modulation of the external potential and its harmonics. It is through these modes with wave vectors in the x direction (j) that energy is transferred to the phonons. After this, however, [Figs. 9(c), 9(d), 10(c), and 10(d)] the energy predominantly spreads into wave vectors with a y component ($l \neq 0$). This channel of dissipation does not exist in the 1D models.

The pattern in which the energy spreads out depends strongly on the elastic parameters, stretching out (compressing) in the y direction for lower (higher) K_{shear} or ξ . For the scalar model in particular, it is clear from Eq. (8) that the phonon dispersion level curves transform similarly, which indicates that energy is most easily spread between modes with comparable frequencies. This explains the general decrease in friction with K_{shear} seen in Fig. 8(a), as the minimal gap in frequency between neighboring modes is inversely related to K_{shear} . We suspect that a similar effect is at play in the vector model.

For the scalar model, the second polarization (y) is inconsequential due to the decoupling, as can be seen from Figs. 9(b), 9(d), and 9(f). The vector model (Fig. 10), however, does have coupling between x and y dynamics, which opens up yet another channel for dissipation: here energy is also appreciably transferred to the y polarized phonon modes. The vector model is thus, with its coupled equations of motion, capable of dissipating energy throughout the 2D spectrum with respect to both the wave vector and polarization.

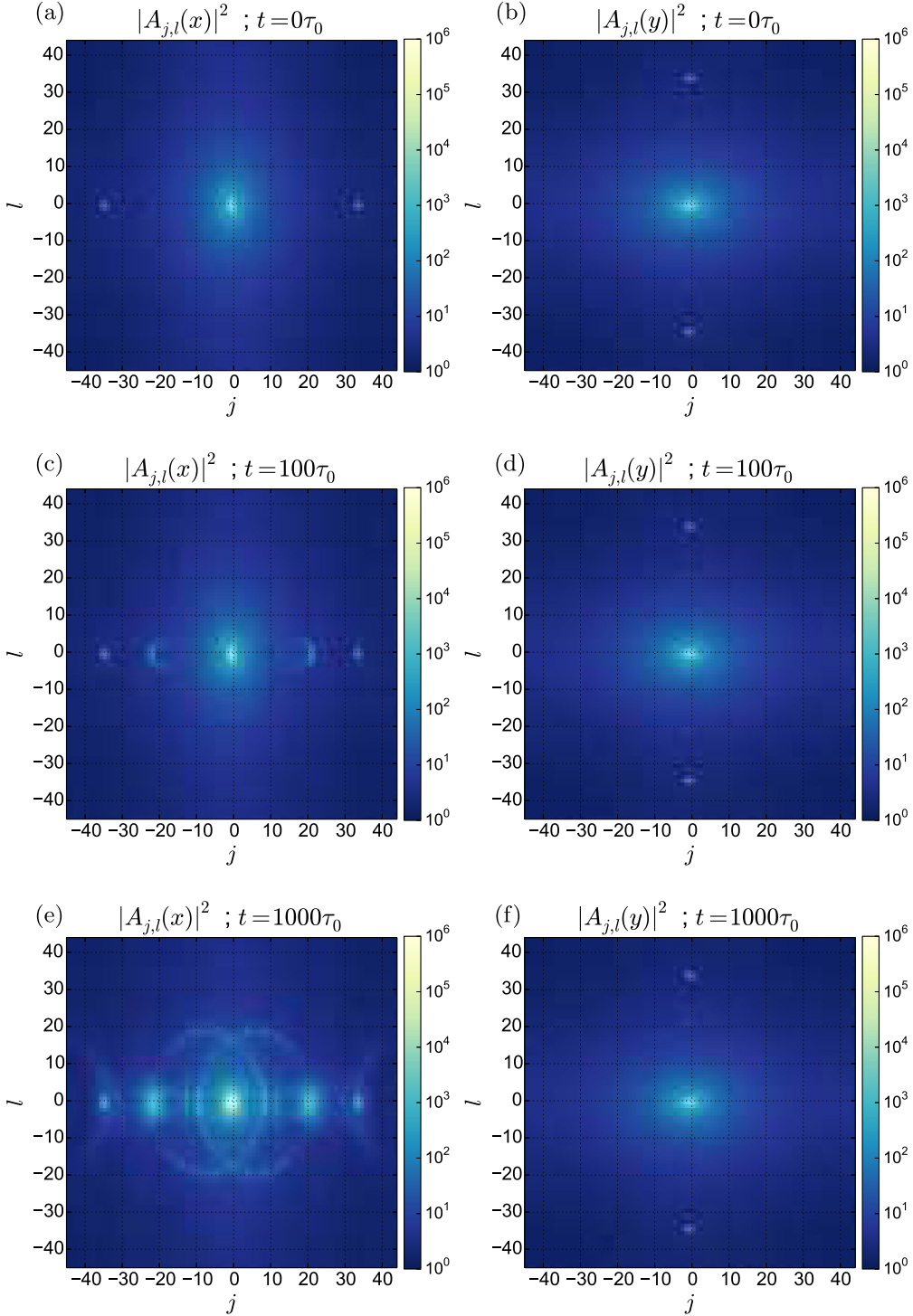


FIG. 9. The population of the phonon modes starting from initial temperature $T = 0.022\lambda$ as a function of time for the scalar model with $K_{\text{shear}} = 0.5$. The squared modulus of the Fourier transformed coordinates $A_{j,l}(x)$ (a, c, e) and $A_{j,l}(y)$ (b, d, f) is plotted at different times after the velocity increment $v_x^+ = 0.12$.

VII. TWO-DIMENSIONAL EFFECTS ON THE VISCOUS FRICTION

On the basis of the above results we conclude that a suitable extension of the FK model to two dimensions for describing sliding friction is the vector model with $\xi = 0.33$ (hereafter referred to as the 2D model). In this section we show some of the new effects which occur in two dimensions. All

calculations follow the same procedure as in Sec. V, where not otherwise stated.

A. Temperature dependence

We first study the dependence of the friction on the initial temperature, as it is ultimately the temperature-induced fluctuations which cause the viscous decay of the CM velocity.

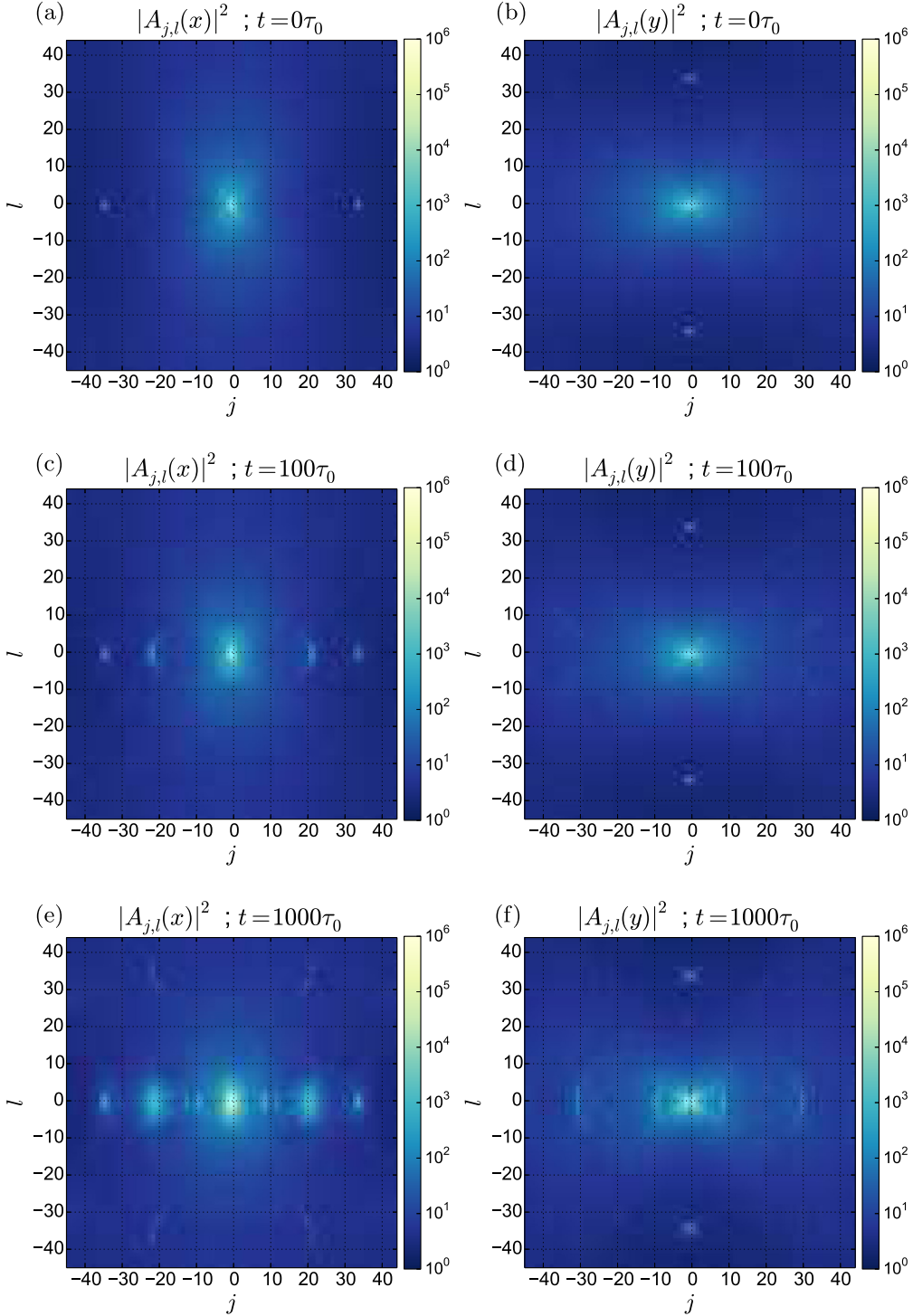


FIG. 10. The population of the phonon modes starting from initial temperature $T = 0.022\lambda$ as a function of time for the vector model with $\xi = 0.33$. The squared modulus of the Fourier transformed coordinates $A_{j,l}(x)$ (a, c, e) and $A_{j,l}(y)$ (b, d, f) is plotted at different times after the velocity increment $v_x^+ = 0.12$.

Shown in Fig. 11 are the friction-velocity curves obtained for the 1D (a) and 2D (b) model for four different values of the initial temperature: $T = 0.022\lambda, 0.063\lambda, 0.12\lambda, 0.16\lambda$. The results for the 1D model are in good agreement with previous results [21]. Increased temperature here leads to a significant thermal broadening of the resonance peaks. The peak corresponding to $n = 3$ sees an increase in friction as it essentially

becomes a part of the larger $n = 2$ peak. This second peak however remains distinguishable, and its maximum value is approximately constant for all temperatures.

For the 2D model we find both similarities and differences to the 1D case. Also in this case the peaks are thermally broadened. However, the effect is smaller, i.e., peak $n = 2$ remains more narrow than in the 1D model. Importantly we

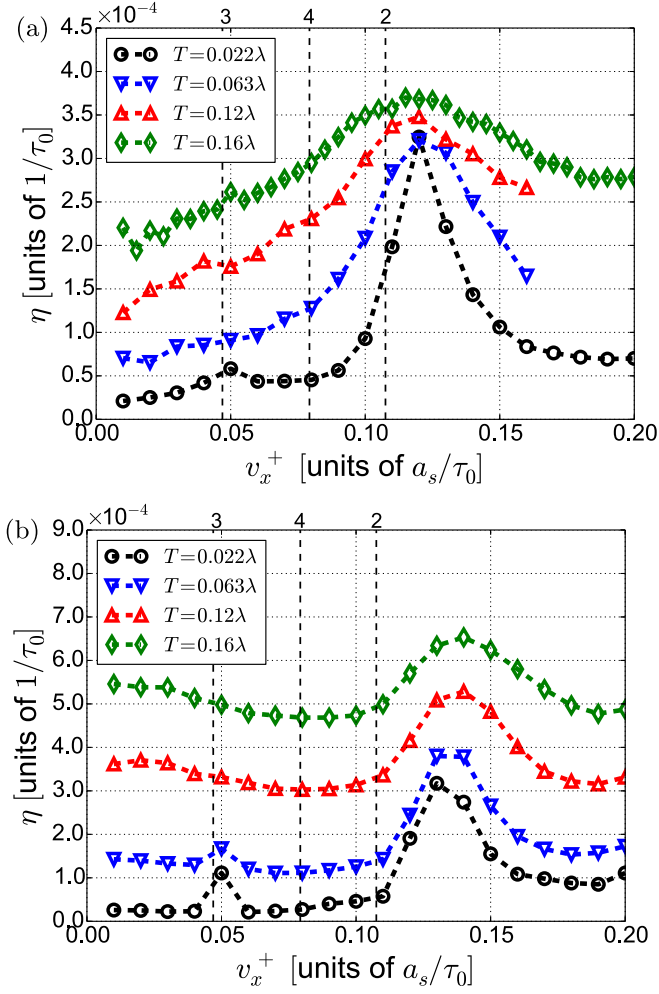


FIG. 11. Viscous friction coefficient η as a function of velocity v_x^+ for the 1D (a) and 2D (b) models and four different temperatures, each corresponding to equilibration from sliding at the first four resonant velocities, as in Ref. [21]. Dashed vertical lines indicate the positions of the second, third, and fourth resonances. The temperature affects the resonance peaks differently in two dimensions.

also observe a shift of all the curves towards higher friction, i.e., the maximum value of the peak does not remain the same. This shift is a qualitatively new behavior which has not been seen in the 1D model.

We note that the values we find for the viscous friction coefficients are significantly lower than those typically found in experiments, which would be around $1/\tau_0$. However, we observe that the temperature-dependence changes dramatically with dimensionality and that the friction increases with dimensionality overall, due to the increase in the number of degrees of freedom which energy can be dissipated into. Thus, we expect that the viscous friction in a 3D model would be substantially larger than it is in our 2D systems.

B. Anisotropy of the sliding direction

For a 2D model, just as in real systems, the sliding is not necessarily restricted to a specific direction. At the atomic scale, the 2D friction force needs not be the same in all directions (see, for example, Ref. [29]), and it can even have

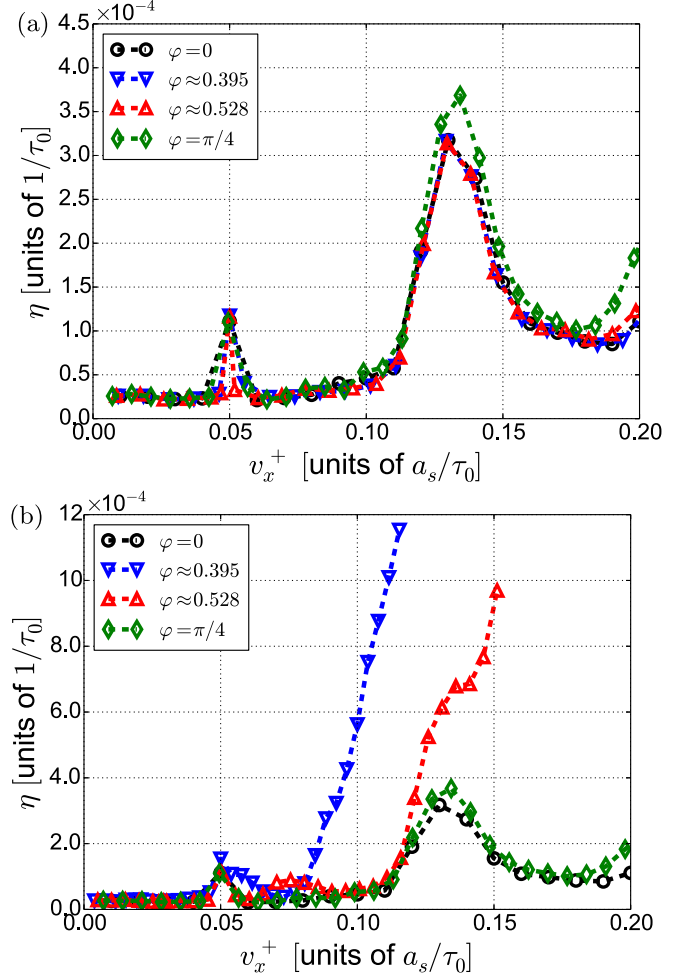


FIG. 12. Friction coefficients η_x (a) and η_y (b) as functions of their respective velocity increment components for angled velocity increments. Results are shown for four different angles $0 \leq \varphi \leq \pi/4$ and initial temperature $T = 0.022\lambda$. Note that the η_x coefficient is shown also in (b) for $\varphi = 0$, as η_y is not a meaningful quantity in this setup.

components perpendicular to the sliding direction (see, for example, Refs. [16,22,30,31]). In this section we therefore show some of the effects of anisotropy which may occur when the velocity increment is not chosen along a symmetry axis.

We use $\vec{v}^+ = v^+(\cos \varphi, \sin \varphi)$, i.e., a velocity increment in a direction φ . The CM velocity then consists of two components $\vec{v} = (v_x, v_y)$ which may potentially decay at different rates. We perform one exponential fit to each component to extract the two friction coefficients η_x and η_y . The fitting procedure is otherwise identical to previous sections. To reduce the number of parameters we consider once again only the low-temperature case $T = 0.022\lambda$. In Fig. 12 we show η_x (a) and η_y (b) for four different angles $0 \leq \varphi \leq \pi/4$, i.e., v_x^+ larger than or equal to v_y^+ .

The behavior of η_x is similar for all four angles. It is only for the case of $\varphi = \pi/4$ (i.e., $v_x^+ = v_y^+$) where a small increase in friction can be found for high velocities ($v_x^+ \gtrsim 0.12$). The friction can thus, in this case, be well described in terms of the single velocity increment component v_x^+ , disregarding to good approximation any influence of v_y^+ .

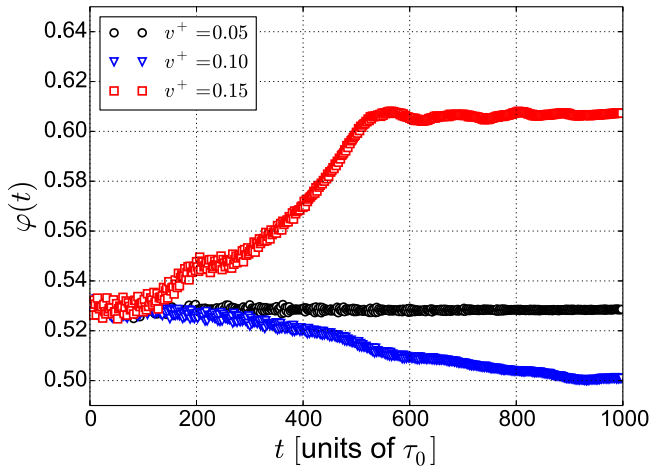


FIG. 13. The sliding angle $\varphi(t)$ as a function of time after three different velocity increment magnitudes v^+ , for initial angle $\varphi \approx 0.528$ and temperature $T = 0.022\lambda$. The direction of the velocity changes, because the friction force is not parallel to the velocity. As a consequence of this, the sliding direction changes depending on the magnitude of the velocity.

As expected, η_y is identical to η_x in the limiting case $\varphi = \pi/4$. For the two smaller angles, however, a significant increase in friction is found for intermediate to high velocities ($v_x^+ \gtrsim 0.06$), as compared to a velocity increment with the same v_y^+ but $v_x^+ = 0$. The sliding in x which has been projected out in Fig. 12(b) couples strongly to the y dynamics. As this additional sliding rapidly raises the temperature, friction becomes much higher. We emphasize that this 2D effect could never arise in the scalar model, as the velocity and friction components would then be individually determined for x and y from the one-component sliding described in Sec. V A.

The possibility for different decay rates in the velocity components also gives rise to an interesting effect when considering the time evolution of the sliding angle $\varphi(t) = \arctan[v_y(t)/v_x(t)]$. In Fig. 13 we show $\varphi(t)$ for three different velocity increment magnitudes and initial value $\varphi \approx 0.528$. Here we see that the angle can, depending on the velocity increment, either remain nearly constant or vary with time. In two dimensions the lattice can thus follow a curved trajectory due to friction forces perpendicular to the sliding direction, instead of a straight line as would be expected macroscopically. For a given initial direction, the magnitude of the velocity can thus be used to control the trajectory.

VIII. CONCLUSIONS

We have examined friction in the FK model in two dimensions, considering the additional parameters that result

from the extra dimension as well as the more complex phonon spectrum when compared to one dimension.

We have systematically investigated how two common types of extensions for the 1D FK model to two dimensions affect the static and dynamic frictional properties, demonstrating clearly that the process of generalization is not trivial. The models behave very similarly (or even identically) to the 1D case in terms of static properties. The dynamical friction properties, however, are more sensitive to the 2D nature of the models. The wrong type of interaction or parameter choices can lead to unphysical dynamics, and unphysical dynamic friction.

The scalar model, though 2D in terms of particle positions and lattice structure, consists in practice of two decoupled 1D systems which do not interact. It cannot therefore describe thermal equilibration, which is crucial for dissipation, and does not capture 2D behavior of dissipation in real physical systems.

The vector model is in every sense a true 2D model, as the higher order terms in internal interaction couple the coordinate components. However, it is important that the elastic parameter ξ is chosen with care. Too small values of ξ give rise to phonon modes with unphysical dispersion and extremely high friction. For the physically realistic parameter values around $\xi = 0.33$, we find a qualitative but not always quantitative agreement with the 1D case for the dynamic friction and no sign of pathologies.

We have used the vector model to study some unique features that result from the true 2D nature of the system. In two dimensions there are extra channels for dissipation: phonon modes with (quasi-)transverse polarization as well as phonons traveling in directions which are not aligned with the sliding. Their influence is seen in the qualitatively different temperature dependence of the dynamic friction, as compared to the 1D case. The new effects would likely be even stronger in a fully 3D model, as, e.g., there are then several transverse phonon branches.

In addition, the possibility of sliding in directions other than the symmetry axes of the substrate has been demonstrated to result in nontrivial anisotropic effects.

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