"Fuse Safety Device" on an Atomic Scale

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We study a nonlinear response of the underdamped generalized Frenkel-Kontorova model (a system of interacting atoms placed into an external periodic potential) on the dc driving force. Both studied variants of the model, one with a transverse degree of freedom, and another with two-dimensional isotropic substrate potential, exhibit an interesting "fuse"-like behavior: at small forces the system is in the regime of *running* kinks with a nonzero conductivity, while at higher forces the system is trapped in an immobile state. This behavior is explained in terms of a dynamical transition between two states of kinks.

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Driven diffusive systems belong to the simplest models of nonequilibrium statistical mechanics. For example, the Frenkel-Kontorova (FK) model [1] (i.e., an atomic chain placed into external periodic potential and driven by the dc force F) has a wide application area in modeling of charge and mass transport in solids, tribology etc. [2–7]. When the force F changes, this system exhibits a complicated (multistep and hysteretic in the underdamped case) transition from the locked state, where the average system velocity $\langle v \rangle$ is zero, to the sliding state, where all atoms move with the maximum velocity $\langle v \rangle \approx F/m\eta$ (here η is the external damping and m is the atomic mass). Various intermediate regimes can be described by resonance phenomena [4,7], and by the moving quasiparticle excitations of the FK model, *kinks* [6].

All the scenarios observed until now have, however, one common feature: the drift velocity $\langle v \rangle$ *monotonically increases* with F. In the present Letter, we report the first, to the best of our knowledge, observation of the *nonmonotonic* scenario, when the system has a nonzero conductivity ($\langle v \rangle \neq 0$) at low forces and becomes locked ($\langle v \rangle = 0$) at higher forces. Generally, to exhibit such a behavior which resembles a "fuse safety device" on an atomic scale, the system should have the following ingredients: (i) the *mobile* ground state, (ii) a close metastable state, which is *immobile* at the same forces, and (iii) with increasing of the applied force F the system should be moved from the mobile state to the immobile one, thus locking itself. Such a situation may in principle be organized in various systems. Here we describe the *fuse* scenario for two simple mechanical models of interacting atoms having *more than one spatial dimension*.

(A) The FK model with a transverse degree of freedom [8], i.e., the chain of atoms of unit mass subjected to the 2D external potential sinusoidal with the amplitude $\varepsilon = 2$ and the period $a = 2\pi$ in the x direction (along the chain), and parabolic in the transverse direction y,

$$V_s(x, y) = 1 - \cos(x) + \frac{1}{2}\,\omega_y^2 y^2. \tag{1}$$

(B) The 2D isotropic FK-type model, i.e., the array of atoms adsorbed on the periodic 2D substrate of the square symmetry,

$$V_s(x, y) = [1 - \cos(x)] + [1 - \cos(y)]. \tag{2}$$

For the model **A** an isolated atom near the potential minima has the frequency of x vibration $\omega_x = 1$, while the frequency of transverse y vibration is given by ω_y. For the model **B** the vibrations near the minima are isotropic, $\omega_x = \omega_y = 1$. If the force is applied along x, the isolated atom starts to slide at the critical force $F_{\rm crit} \equiv \pi\varepsilon/a = 1$.

In both models the motion is governed by Langevin equations,

$$\ddot{\vec{r}}_i + \eta\dot{\vec{r}}_i + \frac{dV_s(\vec{r}_i)}{d\vec{r}_i} + \frac{d}{d\vec{r}_i}\sum_{j\neq i} V_i(|\vec{r}_i - \vec{r}_j|) = \vec{F}, \tag{3}$$

where $\vec{r}_i = (x_i, y_i)$ for the ith atom, and $\vec{F} = (F, 0)$ is the external dc force. We take the exponential interaction between the atoms corresponding to the repulsion of atomic cores, $V_i(r) = V_0 e^{-\beta r}$, where r is the distance, β determines the interaction range (in simulation we used $\beta = 1/\pi$ so that a "diameter" of the atom is 2π), and the amplitude V_0 can be expressed for the sake of convenience as $V_0 = g(\pi e)^2$, where g is the so-called discreteness parameter, $g \equiv V_i''(2\pi)/\omega_x^2$. The periodic boundary conditions are imposed in the x (model **A**) or in both x and y directions (model **B**) in order to fix the atomic density. In the simulation we first look for the minimum-energy state of the system, then adiabatically change the force and measure the average drift velocity $\langle v \rangle$ for a given F.

Let us consider the situation when each potential well is filled with one atom (the commensurate structure), plus some excess atoms are added, which in the ground state form localized compressions, or *kinks*. For example, in

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the model **A**, we place N atoms on the M wells, thus having $N_k = N - M$ kinks in the chain with dimensionless concentration $\theta = N/M$. In the model **B**, this is repeated for every row $y = 2\pi n$, n being an integer.

The kinks are known as the effective mass carriers, since they start to slide at a force much smaller than $F_{\rm crit} = 1$. The specificity of both studied 2D models, by contrast with the one-dimensional FK model, is that the extra spatial dimension allows for the transverse y "orientation" of the kinks. We show here that the increasing force, applied along x, can turn the sliding kinks transversely so that they stop, and the system ends up locked. Our main result, the kink velocity [defined as $v_k = \langle v \rangle N/N_k$] versus the external force F at different frictions η and concentrations θ, is shown in Figs. 1a and 2a for the models **A** and **B** correspondingly. The "fused" behavior can be seen clearly: an initially linear growth of v_k with F saturates as soon as the kinks reach certain critical velocity, followed by the drop of v_k to zero. Figures 1b and 2b reveal that this process is accompanied by the growing transverse y displacements of the atoms. Below we analyze this phenomenon in more detail for both studied models.

Model A.—Even the classical FK model has a rich phase diagram with metastable chaotic states [1], while introduction of the transverse degree of freedom leads to a more complicated picture [8]. Namely, above a certain value of the repulsion g^* the minimal frequency $\Omega_y^{\rm min}$ of the transverse phonon spectrum $\Omega_y(k)$ vanishes, and the *trivial* ground state (linear chain with $y = 0$) bifurcates via second-order transition into the *zigzag* ground state (two subchains with $y = \pm\Delta y$). For the exponential repulsion at $\theta_0 = 1$ the critical g^* is determined from the condition [8] $\omega_y^2 \approx -4V_i'(a)/a$. Thus, for our choice of parameters the commensurate structure is trivial if $g < g^* = \omega_y^2/2$, otherwise it is zigzag-like. At $g < g^*$ the frequency $\Omega_y^{\rm min}$ is given by [8] $\Omega_y^{\rm min} = \Omega_y(\pi) = (\omega_y^2 - 2g)^{1/2}$. Since local repulsive forces in the kink core exceed those in the commensurate structure, the bifurcation takes place locally at a smaller g. Thus, there exists some $g_k < g^*$, such that at $g < g_k$ all the system is in the trivial state, while at $g_k < g < g^*$ the chain is still linear far from the kink, but the atoms in the kink core escape out of the $y = 0$ line. One can roughly estimate g_k for a very discrete chain [9], although the actual picture is more complex. For discrete enough chains ($g < 0.5$), when the kink core consists of two atoms, we found the existence of only one type of the y-distorted kink at $g < g^*$, called the *rhomboid* kink (RK), which is shown along with the *trivial* kink (TK) in the insets in Fig. 3a. RK corresponds to a configuration of two atoms placed in one well with the same x and opposite $y = \pm y_{\rm RK}$ [11]. The transition from the TK to RK (e.g., when g is changed) is of the first order and exhibits hysteresis. We plot the energy difference between RK and TK, ΔE, versus g at a fixed ω_y, and determine g_k from the condition $\Delta E = 0$. An example in Fig. 3b ($\omega_y = 1.3$, so that $g^* = 0.845$) gives $g_k = 0.340 \pm 0.002$, while the estimation [9] is ≈ 0.345. Let us emphasize that both RK and TK correspond to *local minima* of the energy, one of them being *stable* and another *metastable* state, separated by nonzero barrier ϵ along the quasiadiabatic trajectory in the energy landscape (Fig. 3a). At $g < g_k$ the barrier ϵ between the saddle-point configuration $(0.2a, 0.21a)$ and RK is shown in Fig. 3b.

To achieve the fuse scenario, let us chose, e.g., $\omega_y = 1.3$ and $g = 0.31 \lesssim g_k$, so that *TK is the ground state, while RK is a close metastable state* (with $\Delta E = 0.176$ and $\epsilon = 0.035$). We start from the initial configuration with TK's. They begin to slide at a small force $F_{\rm TK} = 0.03$ (Fig. 1a)

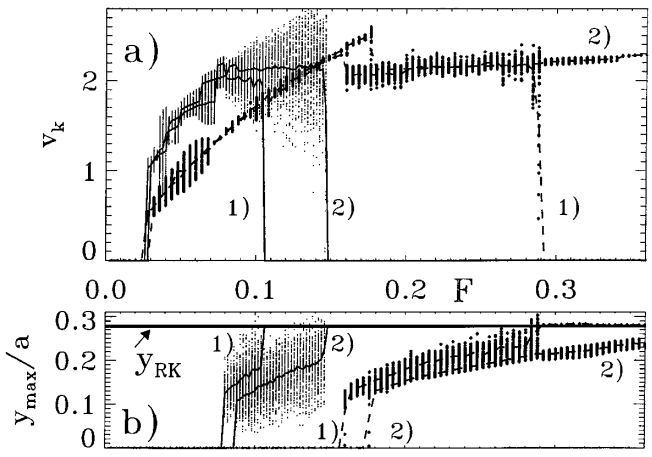

FIG. 1. The fuse scenario in the FK chain with the transverse degree of freedom. (a) The kink velocity v_k versus the force F. Curves show the average values, while symbols are for the raw data from the simulation (100 points taken during the time 200π for each value of F). Small dots and solid curves are for $\eta = 0.1$, bold dots and dashed curves are for $\eta = 0.2$. The label (1) near the curves denotes the $\theta = 64/56$ case, and (2) denotes the $\theta = 64/60$ case. (b) The same as in (a) for the maximum y displacement of the atoms $y_{\rm max}$.

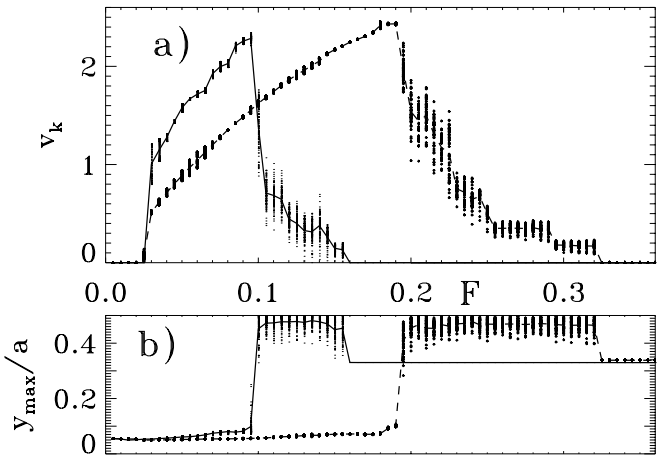

FIG. 2. The fuse scenario for the 2D isotropic FK model. The notation is the same as in Fig. 1. Here we define $y_{\rm max}$ as the maximum deviation of the y coordinate of an atom from the nearest line $y = 2\pi n$, n being an integer.

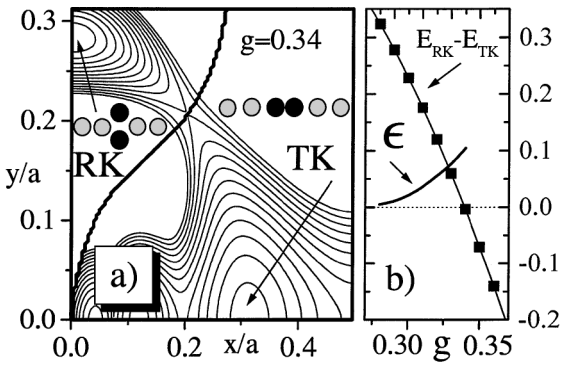

FIG. 3. Trivial and rhomboid kinks in the FK chain with the transverse degree of freedom. (a) The contour plot of the total energy of the system in the (x, y) plane (the interval between levels is 0.01). The energy was measured with one of the atoms in the kink core given a shift (x, y) from the bottom of the well and kept fixed, and the rest of the chain relaxed (see details in [10]). After releasing of all atoms and one more relaxation, we find also the regions of attraction for RK and TK (separated by the bold curve). Insets: The sketches of TK and RK (black circles denote the kink core). (b) The energy difference $\Delta E = E_{\mathrm{RK}} - E_{\mathrm{TK}}$ and the barrier $\epsilon = E_{\mathrm{saddle}} - E_{\mathrm{RK}}$ as functions of g. Both (a) and (b) are for $\omega_y = 1.3$.

needed to overcome the Peierls-Nabarro (PN) barrier ε_{pn} [equal to the energy difference between the points $(0.5a, 0)$ and $(0.31a, 0)$ in Fig. 3a]. By contrast, having chosen the RK's as the initial condition, one does not see any dynamics in the system until a much larger force $F_{\mathrm{RK}} \approx 0.37$, when RK's start to move. Note that the beginning of the motion of RK is not related to the degradation of its PN barrier (the barrier ϵ in Fig. 3), because the path from the equilibrium RK position to the saddle point configuration (Fig. 3a) does not coincide with the x direction, while the force is applied along x.

At the critical velocity $v_c \approx 2.1$ (Fig. 1a) the behavior of sliding TK's changes qualitatively: the atoms *in the cores of kinks* start to oscillate transversely, and the kinks produce y-oscillating decaying tails. With further increase of the force the kink velocities remain fixed at v_c, while the amplitude of y oscillations grows, and when its maximum $y_{\max}$ reaches the equilibrium position for RK $y_{\mathrm{RK}} \approx 0.27a$ (see Fig. 1b), the system locks ($\langle v \rangle = 0$) at a force F_{lock}, where F_{lock} depends both on η and θ. The typical locked atomic configuration consists of *rhomboid* kinks bunched in a compact group (a stopped kink acts as a trap for the kinks behind it). This locked state persists in the range of forces $F_{\mathrm{lock}} < F < F_{\mathrm{RK}}$, i.e., it is destroyed only when RK's start to slide, and the system goes to the totally running state. The locked state with RK's is *metastable*, its energy (after the force is decreased back to $F = 0$) is higher than that for the state with TK's.

In the y-oscillating state just preceding the locking, one can visually distinguish separate kinks, however the overall system dynamics is chaotic. The number of positive Lyapunov exponents in this state is equal to the number of kinks N_k, and the Fourier spectra of both v_x and v_y are continuous with high-frequency tails decaying via a power law $S_v(\omega) \propto \omega^{-5}$ [12]. According to our observations, the chaotization of the kink's motion plays an important role in the fuse scenario, allowing the system to reach eventually, due to chaotic y oscillations, the region of attraction of the RK configuration (Fig. 3a). Indeed, when the kinks dynamics is *regular* (e.g., at higher frictions $\eta > 0.3$) we *never* find the fuse scenario, though the y oscillations may emerge. Note that the force $F \approx 0.1 \div 0.3$ (Fig. 1) is already large enough to gain (at a distance $\sim a/2$) the energy needed for the transition to the RK state, $\Delta E + \epsilon \approx 0.2$ at $g = 0.31$.

Let us discuss the dependence of the locking threshold F_{lock} on η and θ (Fig. 1a). First, the force F_c, when y oscillations emerge at the critical velocity v_c, increases with η and is nearly independent on θ. Indeed, we found that the initial growth of v_k with F follows the dependence $v_k \propto F/\eta$, so that $F_c \propto \eta v_c$. Second, with further increase of the force the condition $y_{\max} \approx y_{\mathrm{RK}}$ is also achieved later at higher frictions (resulting in a larger F_{lock}) because of the smaller amplitude of the chaotic y oscillations (Fig. 1b). Thus, the friction must be low enough to get $y_{\max} \approx y_{\mathrm{RK}}$ at $F_{\mathrm{lock}} < F_{\mathrm{RK}}$. Third, we observed in separate simulations [12] that even for a single kink in a long chain ($\theta = 512/511$) the internal y oscillations become chaotic at low frictions ($\eta < 0.04$), and the fuse scenario still exists. However, the presence of *many* kinks (larger θ) effectively enhances the probability of the transition to the RK state (i.e., it reduces F_{lock} at a fixed η), probably because of the fluctuations of interkink distances (when two kinks come close enough to each other, they locally reduce the energetic barrier needed for the transition to RK).

As the transverse instability of the TK's motion is the main reason for the fuse behavior, let us dwell on it in some more detail. Provided that RK coexists with TK at given g and ω_y this instability can lead to a fuse scenario, but in fact it is observed in a much wider region of the system parameters. At lower frictions the instability results in the chaotic y oscillations, while at higher frictions we can see the regular *antiphase* y oscillations in the core of running kink, with kink's velocity in both cases fixed at a value v_c (independent on η and θ) when the force increases. This indicates that the y instability should have a resonant origin. Furthermore, at larger frictions, when the atomic motion is regular, we found that the propagation of the kink for one lattice constant a corresponds to $1/4$ of the period of the *local* y oscillation of atoms in the kink core, which means that $v_c = 4\Omega_{\mathrm{eff}}$, where $\Omega_{\mathrm{eff}} < \Omega_y^{\min}$ is a *local* y frequency of the antiphase oscillations of the atoms inside the kink. Although we did not determine Ω_{eff} analytically, we found, varying ω_y and g, that v_c is well fitted (both for the regular and irregular y oscillations) with the resonancelike formula $v_c = 4[(\Omega_y^{\min})^2 - C]^{1/2}$ with the constant $C = 0.81$.

Model B.—We placed 225 atoms into the square area of 15×15 unit cells, so that $\theta_0 = 1$. If the interatomic repulsion is not too strong, the atoms are arranged at the bottoms of the wells in the simple $p(1 \times 1)$ structure. Now let us add one extra atom in every x row thus obtaining $\theta = 16/15$, i.e., one kink in each x row (we denote these kinks as the "↔" kink). However, this system allows also another kink orientation (along y, denoted as the "↕" kink), and these two configurations are separated by a nonzero energetic barrier. If we apply a force *along* x, the "↔" kinks start to move (nearly linear growth of v_k with F), but then, at a critical velocity $v_{c2} \approx 2.4$, there occurs a sharp increase of the transverse y oscillations of the atoms in kinks' cores, and the system eventually locks in the state with the "↕" kinks, thus demonstrating the fuse scenario (Fig. 2, the plots of $v_k = 16\langle v \rangle$ versus F for $g = 0.31$ are shown). Note that v_k does not fall sharply as in Fig. 1, but shows instead some gradual decrease. This is related to the decrease of the total number of running kinks, because the transition to the "↕" kinks does not take place in all rows simultaneously. However, the velocity of the running "↔" kinks is fixed at v_{c2}.

The notable difference from the model A (which required some fine tuning of g or ω_y in order to put the system in the region of RK and TK coexistence) is that in the model B the fuse scenario is more *generic*, we observe it in a wide range of system parameters ($g < 1.0$, $\eta < 0.3$). The fuse scenario also takes place in the model B if the initial configuration consists of a mixture of the "↕" and "↔" kinks; when a small spatial anisotropy is introduced ($\omega_y > \omega_x$), so that the "↔" kink is stable and the "↕" kink is metastable; and we observed it as well in a 2D system with the triangular symmetry [12].

In summary, we have found that the underdamped system of interacting atoms placed in an external periodic potential with more than one spatial degree of freedom may exhibit the "fuse" scenario of the dynamical phase transition in response to the dc force. Namely, after an intermediate regime of running kinks with nonzero conductivity, the system can then be trapped in an immobile state. The mechanism of this trapping lies in random transverse oscillations of the atoms in the cores of kinks. When the force grows, the amplitude of these oscillations sharply increases after the kinks reach certain critical velocity, and finally the mobile state is transformed into an immobile one with the kinks oriented *transversely* to the applied force.

Although the fuse scenario assumes a special choice of system's parameters, they are quite typical for such physical systems as, e.g., atoms adsorbed on metal surfaces. The comparatively simple atomic systems with the behavior similar to the "fuse safety device" could be of great interest for the development of various atomic-scale devices. Besides, this scenario can be found in other nonlinear models, e.g., it has been recently reported for the system of two coupled solid state lasers [13].

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[9] If we consider only two (weakly repelling) atoms placed in the same well of the external potential, the pair will align along x (TK) if $\omega_y > \omega_x$, and along y (RK) otherwise. The rest of the chain reduces the minimal y frequency as $\Omega_y^{\min} = (\omega_y^2 - 2g)^{1/2}$, but does not change the minimal x frequency $\Omega_x = 1$. Equalizing $\Omega_y^{\min} = \Omega_x$, we obtain a critical value $g_k \approx (\omega_y^2 - 1)/2$, which fairly well fits with the simulation data as long as $g_k < 0.5$.

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