# JAMMING IN NONLINEAR DRIVEN MODELS

O.M. BRAUN

Institute of Physics, Nat. Acad. Sci. of Ukraine
*(46, Nauky Prosp., Kyiv 03028, Ukraine; e-mail: obraun@iop.kiev.ua)*

UDC 539.9


The driven underdamped system of anharmonically interacting atoms in the periodic 1D and 2D external potential is studied. When the driving force increases, the system transfers from a locked state to an ordered sliding state corresponding to a moving crystal. It is shown that, before the transition to the sliding state, the system passes through an inhomogeneous state, where it splits into regions of immobile atoms ("traffic jams") and regions of running atoms. We propose a new model, where the particles have a complex structure treated in a mean-field fashion: the collisions of particles are inelastic, and each particle is considered as having its own thermostat. When an external force is applied to atoms, this model exhibits a hysteresis and a clustering of atoms (the traffic-jam regime) for a much wider range of model parameters than that in the classical elastic model, and both these effects survive at high temperatures.

## 1. Introduction

Driven diffusive systems belong to the simplest models of nonequilibrium statistical mechanics. These systems are characterized by a locally conserved density, and a uniform external field sets up a steady mass current. The systems of this class have a wide application area in the modeling of charge and mass transport in solids.

Traditionally, the diffusive systems are studied in the framework of discrete lattice-gas models (e.g., see [1] and references therein), while much less is known about the behavior of continuous models. One of the simplest *continuous* diffusive models is the generalized Frenkel—Kontorova (FK) model [2]. In this model, a one- or two-dimensional array of atoms is placed into the external periodic potential, and the atomic current in response to the dc driving force $f$ is studied by solving the Langevin motion equations. The mobility and diffusivity of the FK-type models are determined by kinks (topological excitations corresponding to the local compression or extension of a commensurate structure) [2—4]. The dynamics of an FK system was found to be strongly affected by the damping coefficient $\eta$ in the Langevin equations [2]. For a small applied force $f$, the total potential experienced by a particle possesses an array of local minima. Hence, the particles are in the locked state, and the system mobility $B = \langle v \rangle / f$ vanishes at zero temperature and is exponentially small at low temperatures (here, $v$ is the drift velocity and $m$ is the atomic mass). When $f$ increases, the system behaves in different ways depending on the value of $\eta$. In the overdamped case, $\eta \gtrsim \omega_s$ (here, $\omega_s$ is a characteristic frequency of atomic oscillations at the minimum of the substrate potential), the minima in the total potential vanish at some critical force $f_s$, and the particle begins to slide over the corrugated total potential with almost a maximum mobility of $B = B_f \equiv (m\eta)^{-1}$, so that the system is in the sliding state. On the contrary, in the underdamped case, $\eta \ll \omega_s$, the system may possess a sliding solution even before the minima of the total potential vanish. In the latter case, the function $B(f)$ exhibits a hysteresis. In addition, during the locked-to-sliding transition, the atoms have a tendency to be organized in compact groups of two different types. One consists only of slowly moving atoms (which resemble "traffic jams"), and the other one includes "running" atoms moving with the maximum velocity [2]. The jamming effects have attracted a broad interest in different areas of physics, in particular, in plastic flows of a solid or in the physics of granular gases. In addition, last years, the driven diffusive models are used in tribology, where the driving force emerges owing to the motion of one of two substrates separated by a thin atomic layer. It was recognized that, in many cases, namely the jamming is the main source of the static friction [5]. In the present work, we study numerically the jamming effects in continuous FK-type models. We consider three variants of the model: the 1D FK model with anharmonic interatomic interaction (Sec. 2), the isotropic 2D FK model (Sec. 3), and the "soft" 1D FK model, where interatomic collisions are inelastic (Sec. 4). All these models exhibit phase segregation for some range of model parameters. In Sec. 5 we present a qualitative explanation of simulation results. Finally, Sec. 6 concludes the paper.

## 2. Anharmonic FK Model

As the first example, let us consider an anharmonic FK model. Let a chain of $N$ atoms be subjected to the sinusoidal external potential with the amplitude $\varepsilon = 2$

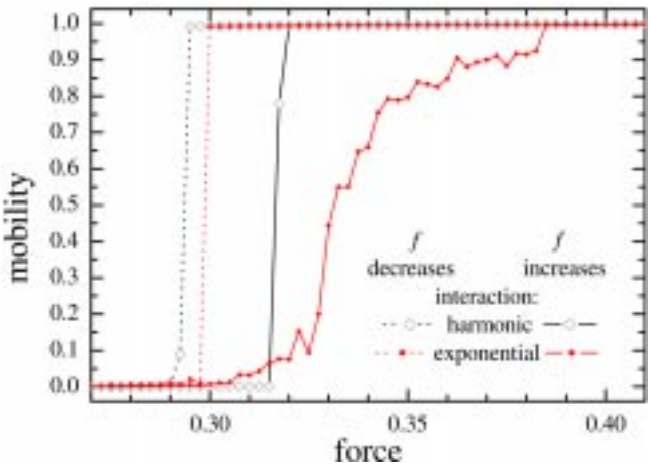


Fig. 1. The dependences $\eta B(f)$ for the standard Frenkel—Kontorova model with harmonic interaction (open diamonds) and for the model with exponential interaction (2) with $\beta = 1/\pi$ (solid diamonds). Solid curves correspond to an increasing force and dotted curves to a decreasing force. The model parameters are $\theta = 2/3$, $N = 256$, $g = 0.1$, $T = 0.1$, and $\eta = 0.1$

and the period $a = 2\pi$, the atomic mass is $m = 1$ (this defines our system of units). The equation of motion for the atomic coordinate $x_l$ reads

$$\ddot{x_l} + \eta\dot{x_l} + \sin x_l + \frac{\partial}{\partial x_l}\left[V(x_{l+1} - x_l) + \right.$$

$$\left. + V(x_l - x_{l-1})\right] = f + \delta F_l(t), \qquad (1)$$

where $1 \le l \le N$, and the periodic boundary conditions are assumed. The substrate potential has $M$ wells on the chain length, so that the dimensionless atomic concentration is $\theta = N/M$, and the average distance between the atoms is $a_A = a/\theta$. The coefficient $\eta$ corresponds to the external viscous damping due to the energy exchange between the chain and the substrate. For the interaction of nearest neighboring atoms, we took the exponential potential

$$V(x) = V_0 e^{-\beta x}, \qquad (2)$$

so that the characteristic radius of interaction is $r = \beta^{-1}$. The dimensionless elastic constant, which is the main parameter of the classical FK model, is defined as [2]

$$g = a^2 V''(a_A)/2\pi^2\varepsilon. \qquad (3)$$

For potential (2), $g$ is equal to $g = V_0\beta^2 \exp(-\beta a_A)$. To all atoms we applied a dc force $f$ and also the Gaussian random force $\delta F_l(t)$, $\langle \delta F_l(t)\, \delta F_{l'}(t')\rangle = 2\eta T \delta_{ll'}\delta(t - t')$, which models a thermal bath with a temperature $T$. In simulations, we calculated the average system velocity and then the mobility $B$ defined as $B = \langle v\rangle/f$, where $\langle \ldots \rangle$ stands for the averaging over the system and time. If the substrate potential is absent, for any $f > 0$ after a time $t \sim \eta^{-1}$ the system reaches a steady state characterized by the maximum mobility $B_f$. In addition, we calculated the velocity correlation function

$$K_v = \langle (\dot{x}_{l+1} - \dot{x}_l)^2 \rangle \qquad (4)$$

which will be used to distinguish a homogeneous steady state from inhomogeneous ones.

The simulation results are presented in Fig. 1.

Comparing the hysteretic curves of Fig. 1 for the standard FK model (open diamonds) with those calculated for the exponential interaction (solid diamonds), one can see the following essential difference between them. For the harmonic interaction, the system goes directly from the low-mobility (locked) state to the high-mobility (running, or sliding) state. Although the system may be found in steady states with intermediate values of $B$, these states always correspond to a *homogeneous* state on a spacial scale larger than the lattice constant $a$. On the other hand, for an anharmonic interaction between the atoms, the system passes through intermediate states which are *spatially inhomogeneous*. In this type of steady states, the system splits into two qualitatively different regions which differ by the atomic concentration and velocities. A typical picture of atomic trajectories is presented in Fig. 2.

One can clearly distinguish "running" regions, where atoms move with almost maximum velocities, and "traffic-jam" regions, where atoms are almost immobile. The regions characterized by a larger atomic concentration and smaller (almost zero) atomic velocities are called by *jams* in what follows. Figure 2 also demonstrates the dynamics of a single jam. The jam grows from its left-hand side due to incoming atoms which stop after collisions with the jam and then join the jam. From the right-hand side, the jam shortens, emitting atoms to the right-hand-side running region. In addition, one can see also a detailed scenario of the jam's dynamics: when an incoming atom collides with the jam, it creates a kink (local compression) in the jam. This kink then runs to the right-hand side of the jam and stimulates there the emission of the atom into the right-hand-side running domain.

Thus, the simulations show that the traffic-jam state may correspond to a steady state of the system. A detailed numerical analysis [6] combined with the investigation of the corresponding Fokker—Planck

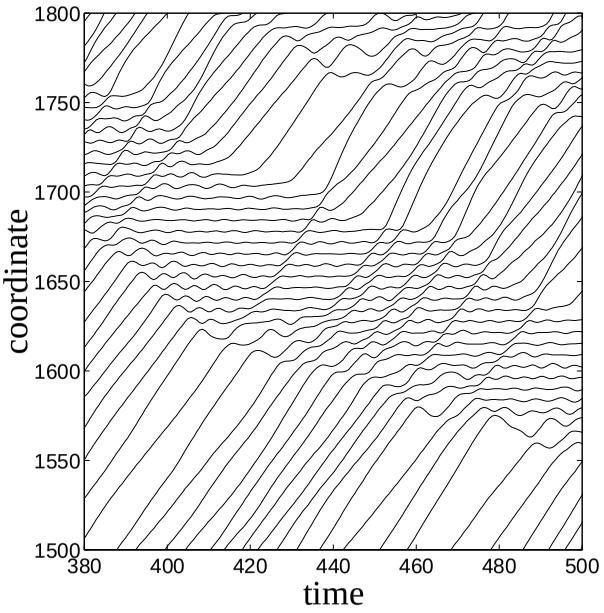


Fig. 2. Atomic trajectories for the 1D FK model with exponential interaction with $\beta = 1/\pi$ at the fixed force $f = 0.33$. The model parameters are $\theta = 2/3$, $N = 256$, $g = 0.1$, $T = 0.1$, and $\eta = 0.1$

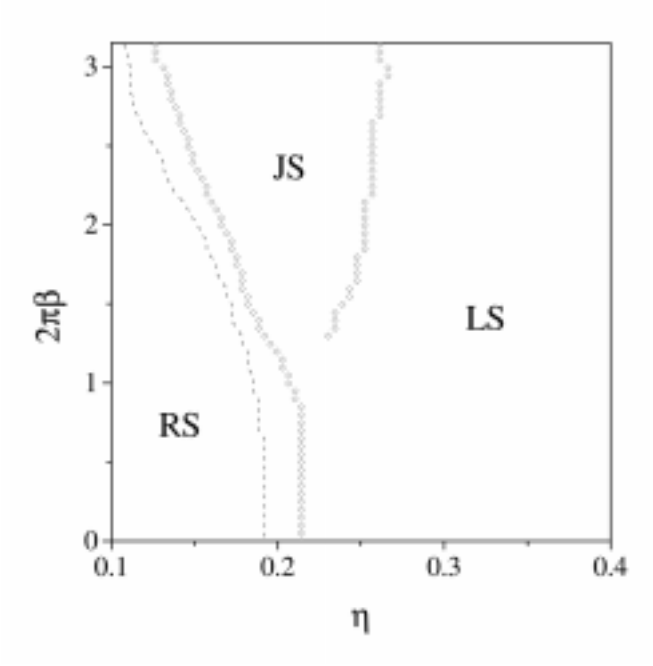


Fig. 3. Phase diagram on the $(\eta, \beta)$-plane. LS is the locked state, JS is the steady state with jams, and RS is the running state. Diamonds correspond to maxima of the correlation function $K_v(\eta)$, and the dashed curve corresponds to the $B(\eta) = 0.9\, B_f$ threshold. The diagram was constructed by varying $\eta$ for different values of the exponent $\beta$ at a fixed value of the elastic constant $g = 0.1$ and the driving force $f = 0.5$. Other model parameters are $\theta = 2/3$, $N = 256$, and $T = 0.1$

equation confirmed that the $T = 0$ state with traffic jams corresponds to the strange attractor of the system and, moreover, the traffic-jam state remains stable at nonzero temperatures, at least for small enough temperatures.

The existence of jams could be expected only for the *underdamped* system, because the system must have two different states for atoms, the running state and the locked state, and this is possible only when $\eta < \eta_c \simeq \pi^2 \varepsilon^{1/2}/4am^{1/2} \approx 0.56$. To study a role of damping, we varied the coefficient $\eta$ keeping the constant driving force $f = 0.5$ and calculating the velocity correlation function (4). When $\eta$ decreases, the system passes from the low-mobility locked state (LS) to the high-mobility running state (RS). For the FK model with harmonic interaction, this transition occurs in one step, and the correlation functions exhibit a peak just at the transition point. For the exponential interaction, the transition may proceed in two steps: First, the system passes to an intermediate state characterized by a plateau with $0 < B < B_f$, and only then, with a further decrease of $\eta$, the running state with $B \approx B_f$ is finally reached. This intermediate state always corresponds to the steady state with jams. At the same time, the function $K_v(\eta)$ exhibits two peaks, one at the transition to the inhomogeneous traffic-jam state (JS), and the second at the transition to the running state. One can see from (4) that the value of $K_v$ should be proportional to the number of jams in the system because the velocities of nearest-neighboring atoms may differ essentially only at the boundaries separating the running and jam domains. Therefore, we can use the fact of the existence of two peaks on the dependence $K_v(\eta)$ as an indication of the jam state, while the positions of these peaks show the parameter range for the JS existence. In addition, to study also a role of the anharmonicity of the interaction, we made a series of runs for different values of the parameter $\beta$, keeping, at the same time, the value of the elastic constant $g$ fixed, so that the limit $\beta \to 0$ corresponds to the harmonic interaction (the standard FK model), while the limit $\beta \to \infty$ describes a hard-core gas. The simulation results are shown in Fig. 3, where we plot the phase diagram on the $(\eta, \beta)$-plane by extracting the positions of maxima of $K_v(\eta)$ for every value of $\beta$.

We come to the conclusion that the traffic-jam state emerges for a short-range interatomic interaction only, when the radius of interaction is smaller than the period

of the external periodic potential [i.e., for $\beta > a^{-1}$ for the exponential interaction (2)], and only for a narrow interval of damping coefficients around $\eta \sim 0.2$.

## 3. A Two-dimensional FK Model

Next, let us consider the two-dimensional Frenkel—Kontorova model. Let a two-dimensional array of atoms with position vector $\mathbf{u} = (u_x, u_y)$ be subjected to a periodic substrate potential with the triangular symmetry, which is a generic example of isotropic 2D systems. The substrate potential is chosen in a simple form

$$V_{\rm sub}(x,y) = \frac{1}{2}\varepsilon \left\{1 - \cos\left(2\pi x/a_x\right)\cos\left(\pi y/a_y\right) + \right.$$

$$\left. + \frac{1}{2}\left[1 - \cos\left(2\pi y/a_y\right)\right]\right\}, \qquad (5)$$

where $a_x = a = 2\pi$ and $a_y = a\sqrt{3}/2$ are the lattice constants. Function (5) is characterized by the isotropic minima organized into the triangular lattice and separated by isotropic energy barriers of height $\varepsilon = 2$. The frequencies of atomic vibrations at the minima are isotropic, $\omega_x = \omega_y = \omega_s \equiv (\varepsilon/2m)^{1/2}(2\pi/a) = 1$. Flat maxima of potential (5) are organized into a honeycomb lattice.

As above in Sec. 2, we consider the case of an exponential interaction between atoms, $V(r) = V_0 \exp(-\beta r)$, where $\beta^{-1}$ is the radius of interaction (in the simulation, we chose $\beta = a^{-1}$). Then the main parameter of the FK model is the effective elastic constant $g = a^2 V''(r_0)/2\pi^2\varepsilon$, where $r_0$ is the average interatomic distance [2]. This single dimensionless number gives an indication of the strength of the elastic constant of the atomic layer relative to the strength of the substrate potential. A value of $g$ much smaller than 1 indicates a weakly coupled layer. This situation may correspond, for example, to a monolayer adsorbed on a crystal surface. A value $g \gtrsim 1$ describes a stiff atomic layer compared with the substrate depth. For example, the case of dry friction between two blocks of material corresponds to this limit.

The equation of motion for the displacement vector $\mathbf{u}_l$ $(1 \le l \le N)$ is given by the Langevin equation

$$\ddot{w}_l + \eta\dot{w}_l + \frac{d}{dw_l}\left[\sum_{l'\ (l'\neq l)} V\left(|\mathbf{u}_l - \mathbf{u}_{l'}|\right) + V_{\rm sub}\right] =$$

$$= f^w + F^w_{\rm rand}, \qquad (6)$$

where $w = u_x$ or $u_y$. The force $f^w = f^x$ or $f^y$ is the externally applied force, while $F^w_{\rm rand}$ is the Gaussian random force required to equilibrate the damped system to a given temperature $T$. In the present work, we modeled the atomic layer by $N = 768$ atoms placed onto the triangular substrate of size $M = M_x M_y = 32 \times 32 = 1024$, so that the dimensionless concentration is $\theta = 3/4$, and we consider a driving force acting in the $x$ direction only, so that $f^x = f$ and $f^y = 0$.

With increase in the driving force for the underdamped system, we always observed a transition from a locked state to an ordered sliding state of *a moving crystal*. However, the scenario of the locked-to-sliding transition and the intermediate phases through which the system passes during the transition, are strongly determined by the values of $g$, $\eta$ and $T$. In most cases, the system passes through *the plastic phase*, where different portions of the lattice are moving with different velocities, or some are moving, while others remain pinned. The plastic phase can be in the form of channels that we call *the plastic channel phase* (this phase is observed both in underdamped and overdamped systems), or in the form of immobile regions in the sea of running atoms that we call *the traffic-jam* (TJ) *plastic phase*. In the plastic channel phase only one part of particles is mobile while others remain pinned for the extremely long time. In the simulation one can observe the channels of crystalline or disorder flow separated by the channel of immobile particles [7]. In the TJ plastic phase, all particles are mobile but, at any moment, a subset of particles spends some short time to be pinned and then continues to move again. These pinned regions look as entities that migrate in the direction opposite to the driving force.

The TJ phase may emerge in the underdamped system only [8]. Figure 4 demonstrates a typical example of the dependence of the mobility $B$ on the driving force $f$ for the stiff layer with $g = 0.857$ for the low damping $\eta = 0.1$.

An intermediate phase appears at $f \approx 0.12$ when the system goes from the pinned state to the disordered steady state with low mobility $B \approx 0.1$. At this phase, the atoms move chaotically around their pinning sites. Looking on atomic trajectories (Fig. 5), we see that this state corresponds to the TJ plastic regime with immobile islands surrounded by regions of slowly running atoms [7].

The TJ steady state survives until the driving force $f \approx 0.34$. Then the mobility increases and the system transfers to the ordered phase of a moving crystal, passing through the plastic-channel regime.

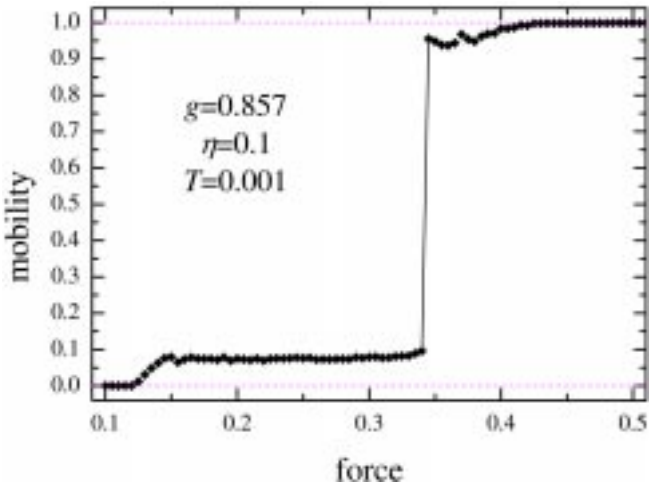


Fig. 4. The normalized mobility $B/B_f$ as a function of driving force for the 2D FK model with $\theta = 3/4$, $g = 0.857$, $\beta = 1/2\pi$, and $\eta = 0.1$ at $T = 0.001$

For a larger damping $\eta = 0.3$, we also observed the plastic TJ flow for $0.23 < f < 0.54$ when $B \approx 0.25$, but now the atomic motion is essentially one-dimensional along channels in the driving direction [7]. The moving atoms strongly oscillate in the transverse direction but remain within their rows. The motion inside each row is similar to the 1D TJ motion in the anharmonic 1D FK model described above in Sec. 2: inside a row, the system splits into closely packed immobile 1D islands (traffic jams) and less dense running domains.

## 4. An Inelastic FK Model

As a third example, let us consider a problem of modeling of a system consisting of "complex" particles which have their own structure with internal degrees of freedom. The internal modes may be excited due to interparticle collisions and take away the kinetic energy of the translational motion, so that the collisions are inelastic. This is a typical situation in soft-matter physics, for example, in the physics of granular gases [9, 10]. A model of such type have been studied recently in [11], where the simplest case of two "atoms" in the double-well external potential was considered, when the atomic hard-core collisions are inelastic. The model exhibits the effect of atoms' "clustering", when both atoms prefer to stay in the same well of the substrate potential and hop simultaneously over the barrier. The model [11] is, however, physically artificial in the sense that it violates the energy conservation principle: the energy which is lost in collisions disappears then forever. As a result, the

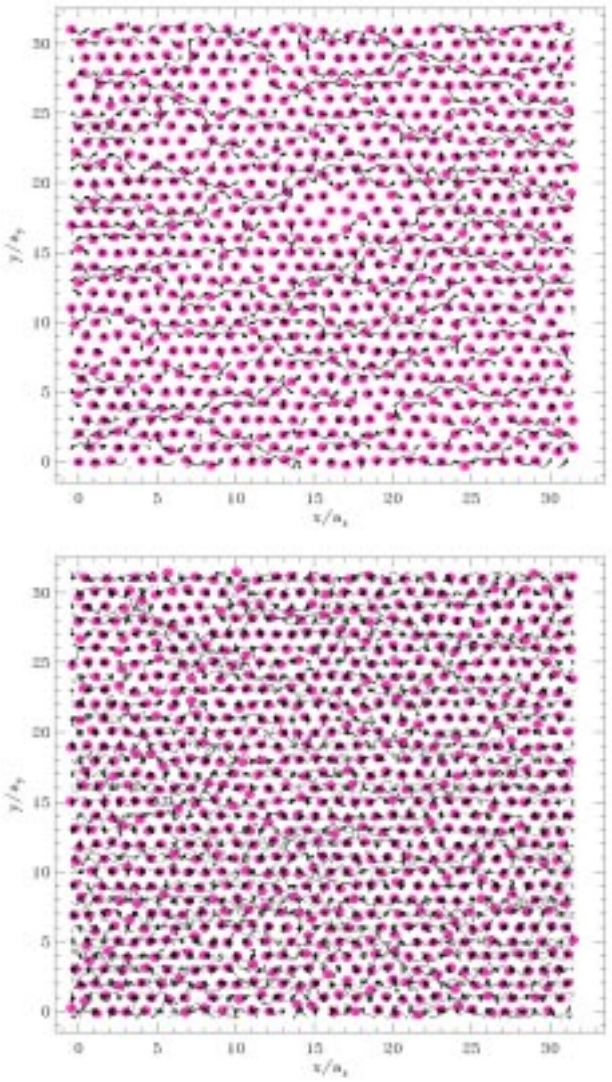

Fig. 5. Snapshot configurations of the TJ plastic phase of the 2D FK model for $g = 0.857$, $\beta = 1/2\pi$, $\eta = 0.1$, and $T = 0.001$ at $f = 0.165$ (top panel) and $f = 0.33$ (bottom panel). Solid curves show atomic trajectories

energy losses due to collisions lead to the effective cooling of the system.

In a more realistic physical model, the kinetic energy of atomic translational motion that is lost at a collision, is stored as the energy of excitation of internal degrees of freedom and may be released later, being transformed back into the kinetic energy. In a simple case, when the number of internal degrees of freedom is "large" and their coupling is nonlinear, the energy lost at collisions is transformed into "heating" of particles. In what follows, we introduce a new type of stochastic models, *the*

*model with multiple thermostats*, where, additionally to the standard "substrate" thermostat, each particle is considered as having its own "thermostat".

As an example, let us again consider the 1D FK-type model with nearest-neighbors (NN) inelastic interaction. Namely, let the chain of $N$ atoms be subjected into $M$ minima of the sinusoidal substrate potential with periodic boundary conditions, so that the motion equation for the $l$th particle has the form

$$m\ddot{x}_l + m\eta\dot{x}_l + \sin x_l = -f_{l+1,\,l} + f_{l,\,l-1} + \delta F_l(t) + f, \quad (7)$$

where the dot (prime) stands for the time (spatial) derivative. To each atom, we apply the dc force $f$ and the viscous damping force with the coefficient $\eta$ which describes the energy exchange with the substrate. The substrate thermostat is modeled by the Gaussian stochastic force $\delta F_l(t)$.

The interaction is taken as exponentially decaying with the interatomic distance, $V(x) = V_0 \exp(-\beta x)$. The inelasticity of collisions is modeled by a viscous damping force proportional to the relative velocity of two atoms, so that the mutual interaction between the $l$-th and $(l-1)$-th particles is described by the force $f_{l,\,l-1}$,

$$f_{l,\,l-1} = -V'(x_l - x_{l-1}) - m_r\eta_l\,(\dot{x}_l - \dot{x}_{l-1}) + \delta f_l(t), \quad (8)$$

where the first term on the r.h.s. of Eq. (8) describes the elastic interaction, $V'(x) \equiv dV(x)/dx$, the second term describes the inelasticity due to viscous damping with a coefficient $\eta_l$, $m_r = m/2$ is the reduced mass of two colliding atoms, and the last term is the stochastic force that compensates the energy losses emerged due to the inelasticity,

$$\langle \delta f_l(t)\ \delta f_{l'}(t')\rangle = 2\eta_l m_r T \delta_{ll'}\delta(t-t'). \quad (9)$$

The mutual damping $\eta_l$ was chosen to depend on the distance between the NN atoms in the same way as the potential, $\eta_l = \eta^* \exp[-\beta(x_l - x_{l-1} - a_A)]$, where $\eta^*$ is a parameter which characterizes the inelasticity: the interaction is elastic in the case of $\eta^* = 0$, while the collisions are totally damped in the limit $\eta^* \to \infty$.

The set of Langevin equations (7)—(9) is equivalent to the Fokker—Planck—Kramers equation for the distribution function $W(\{x_l\},\{\dot{x}_l\};t)$,

$$\frac{\partial W}{\partial t} + \sum_l \left\{ \dot{x}_l \frac{\partial W}{\partial x_l} + [f - V'_{\rm sub}(x_l) + \right.$$

$$\left. + V'(x_{l+1} - x_l) - V'(x_l - x_{l-1})]\,\frac{\partial W}{\partial \dot{x}_l} \right\} =$$

$$= \frac{1}{2}\sum_l \frac{\partial}{\partial \dot{x}_l}\left[ (2\eta + \eta_{l+1} + \eta_l)\left(\dot{x}_l + T\frac{\partial}{\partial \dot{x}_l}\right) - \right.$$

$$\left. - \eta_{l+1}\left(\dot{x}_{l+1} + T\frac{\partial}{\partial \dot{x}_{l+1}}\right) - \eta_l\left(\dot{x}_{l-1} + T\frac{\partial}{\partial \dot{x}_{l-1}}\right)\right] W. \quad (10)$$

It is easy to check that, in the nondriven case where $f = 0$, the Maxwell-Boltzmann distribution is a solution of Eq. (10), so that *our model has the truly thermodynamically equilibrium state.*

In the driven case, $f > 0$, the equilibrium state is destroyed, and the system exhibits a transition from the locked state at low driving (with exponentially low mobility at low temperatures) to the sliding (running) stationary state at high driving, where all atoms move with almost the same velocity $f/m\eta$. For the classical FK model described in Sec. 2, when the interactions are elastic, the average velocity of atoms as a function of $f$ exhibits a hysteresis at zero temperature. But, at any $T > 0$, the hysteresis disappears for an adiabatically slow change of the driving in the 1D model (in simulations, where the force $f$ changes with a finite rate, a small hysteresis persists due to a delay in the formation of the steady state). In addition, in the case of exponential interactions, the steady state during the locked-to-sliding transition for some range of model parameters corresponds to the TJ state with a nonuniform spatial distribution of atoms.

In what follows, we show that both these properties of the transition change drastically for the inelastic interaction. First, the system exhibits a hysteresis even at very high temperatures. Second, the TJ regime is observed for a much wider range of model parameters, thus now it is a generic property of the system. Both these effects appear because of the clustering of atoms: in the case of the inelastic interaction, the energy losses are minimal when the NN atoms move with the same velocity and the mutual viscous forces are zero.

In the simulation, we chose $N/M = 144/233$ which is close to the "golden-mean" atomic concentration. The force was typically changed with the rate $R \equiv \Delta f/\Delta t = 0.0025/(2\cdot 1000\cdot 2\pi) \approx 2\cdot 10^{-7}$ which is low enough to be considered as adiabatically slow. Typically, we used the following parameters: $\eta = 0.01$ (recall that, for the "elastic" FK model, Sec. 2, TJs are observed for a window of frictions around $\eta \sim 0.2$, i.e. for much higher values of the atom-substrate damping), $\beta = 1/\pi$ so that the dimensionless anharmonicity parameter is $\beta a_s = 2$ (according to Sec. 2, TJs appear only for a large enough anharmonicity of the interaction, $\beta a_s > 1$), $g = 1$ (recall that in the classical FK model at $T = 0$, the Aubry locked-to-sliding transition takes place with increase in

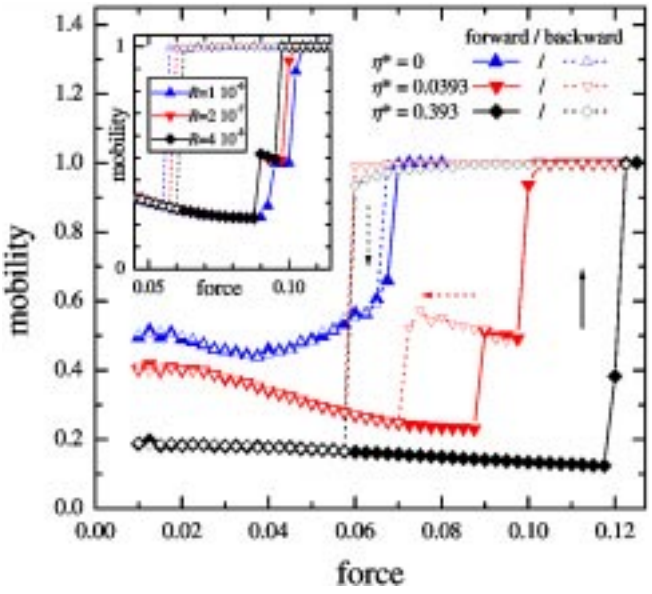


Fig. 6. Dependence of the normalized mobility $B/B_f$ on the force $f$ for three values of the intrinsic damping: $\eta^* = 0$ (up triangles, the elastic model), $\eta^* = e^{-a_A} \approx 0.0393$ (down triangles), and $\eta^* = 10\, e^{-a_A} \approx 0.393$ (black diamonds) for the force increasing (solid curves and symbols) and the force decreasing (dotted curves and open symbols). Other parameters are the following: $\beta = 1/\pi$, $g = 1$, $\eta = 0.01$, and $T = 1$. Inset: $B(f)$ for $\eta^* \approx 0.0393$ for three values of the rate of force changing: $R \approx 10^{-6}$ (up triangles), $R \approx 2 \cdot 10^{-7}$ (down triangles), and $R \approx 4 \cdot 10^{-8}$ (black diamonds)

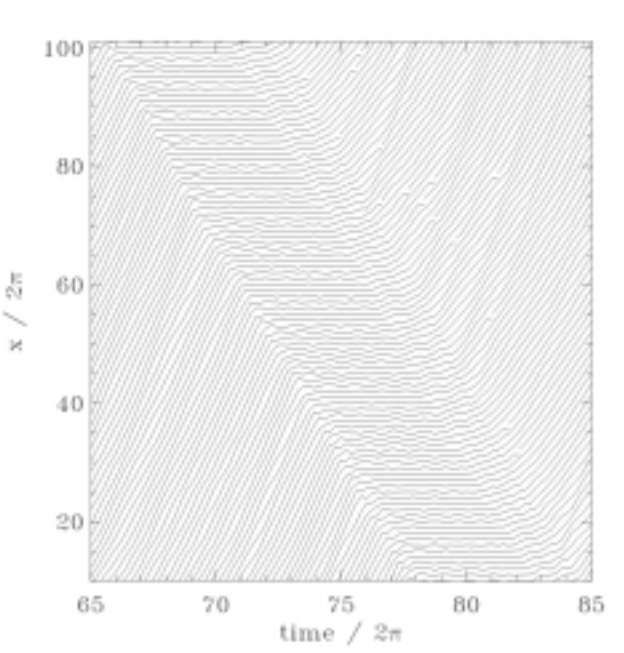


Fig. 7. Atomic trajectories versus time in the traffic-jam regime for $f = 0.095$, $\eta^* \approx 0.0393$, $\beta = 1/\pi$, $g = 1$, $\eta = 0.01$, and $T = 1$

$g$ at $g \approx 1$), and $T = 1$ which is quite large as compared with the barrier height $\varepsilon = 2$.

The simulation results for the normalized mobility $B$ are presented in Fig. 6. One can see that while there is no hysteresis of the $B(f)$ dependence for the elastic model (a narrow hysteresis is because of a finite step of force changing), the hysteresis does exist for $\eta^* > 0$ and its width strongly increases with $\eta^*$. Moreover, the width of the hysteresis does not change essentially if the force increasing/decreasing rate changes by 25 times as shown in the inset in Fig. 6.

We emphasize that the hysteresis in Fig. 6 is for a quite large temperature $T = 1$. Although the hysteretic width decreases when $T$ grows, it still survives even at $T = 2$ (when $\varepsilon_s/k_BT = 1$!) and disappears at huge temperatures only. For example, in the $\eta^* \approx 0.0393$ case the dependence $\Delta F(T) = f_{\text{forward}}(T) - f_{\text{backward}}(T)$ may be fitted by the exponential dependence $\Delta F(T) = \Delta F_0 e^{-T/T^*}$ with $\Delta F_0 \approx 0.156$ and $T^* \approx 0.76$. Therefore, the hysteresis disappears when $\Delta F(T) \lesssim \Delta f = 0.0025$ which gives $T_m \gtrsim 3.15$.

Qualitatively the existence of hysteresis may be explained in the same way as in [6]: The system cannot be transformed from the locked state to the running state and vice versa as a whole; first, a small cluster of atoms (a critical "nucleus") should undergo the transition, and then it will move the whole system into a new state. In the "soft" model considered here, when a fluctuation of the relative velocity of the NN atoms is suppressed, the probability of the emerging of a nucleus with a maximum velocity on the background of immobile atoms (as well as the nucleus of locked atoms in the sea of running ones) is much lower than that in the elastic model.

The hysteretic behavior described above clearly indicates the clustering of atoms in the soft model. One more indication of this effect is the plateau at $B \sim 0.5$ on the $B(f)$ dependence (Fig. 6) which corresponds to the traffic-jam regime. The TJ state appears for the interval of forces $0.09 \leq f \leq 0.0975$ in the force-increasing process and survives till $f \geq 0.0725$ if the force decreases starting from the TJ state. The atomic trajectories in the TJ state are shown in Fig. 7.

Note that now the TJ phase is observed for a much wider range of model parameters and very high temperatures.

To study the TJ state, we calculated the coordinate and velocity correlation functions for the NN atoms, $K_x = \langle (x_l - x_{l-1} - a_A)^2 \rangle$ and $K_v = \langle (\dot{x}_l -$

$\dot{x}_{l-1})^2\rangle$. For a spatially homogeneous state, we should have $K_x \approx K_{x0} = T/g$ and $K_v \approx K_{v0} = 2T$, while, for an inhomogeneous (TJ) state, much higher values are expected. The calculated dependences clearly demonstrate the destruction of the homogeneous state in the TJ regime. However, the TJ state is a more subtle effect of clustering than the hysteretic behavior of the $B(f)$ dependence. For example, for the parameters used in Fig. 6, the TJ state disappears at low damping ($\eta^* = 0$) as well as at too high values of $\eta^*$ (e.g., for $\eta^* = 0.4$).

## 5. Discussion

The TJ state may emerge in an underdamped system only, when the substrate damping $\eta$ is low enough, $\eta < 0.56$, and an atom exhibits bistability, i.e. both states, the locked state and the running state, coexist (and are dynamically stable) at the same driving $f$. Then the locked-to-sliding transition should always pass through the TJ state, and the only question emerges, is this TJ state dynamically stable. To describe qualitatively the steady state with coexistence of two phases in the 1D model, i.e., the TJ phase consisting of locked atoms and the running domain (RD), let us suppose that there is only one jam in the chain, and let the jam contains $N_s$ atoms on the length $L_s = M_s a_s$, while the running domain contains $N_r = N - N_s$ atoms on the length $M_r a_s = (M - M_s)a_s$. According to Figs. 2 and 7, the local concentration in the jam is $\theta_s \equiv N_s/M_s \approx 1$. The atoms in the RD are characterized by a local concentration $\theta_r \equiv N_r/M_r < 1$, and all these atoms move with a velocity $v_r \approx v_f = f/m\eta$. Then it is easy to show [6, 12, 13] that the normalized mobility is equal to $B = N_r v_r/N v_f = b\theta_r(1-\theta)/(1-\theta_r)\theta$, where $b = v_r/v_f \approx 1$.

The TJ grows from its left-hand-side with the rate $R_+ = \dot{M}_s = v_r/a_r$, where $a_r = a_s/\theta_r$, so that $R_+ = b\,\theta_r f/m\eta a_s \leq b\,\theta f m\eta a_s$. From its right-hand-side, the TJ shortens with the rate $\alpha(f)$ due to the "evaporation" of the most right atom of the TJ into the RD. At a low temperature and driving force, when $\varepsilon(f) \approx \varepsilon_s - f a_s/2 \ll T$, the "evaporation" of the most right atom of the TJ is an activated process, and its rate is $\alpha(f) \approx \alpha_0 \exp\left[-\varepsilon(f)/T\right]$, where $\alpha_0$ is a pre-exponential factor. Thus, the TJ decreases with the rate $R_- = \alpha(f) = \alpha_0 \exp\left(-\varepsilon_s/T\right) \exp\left(f a_s/2T\right)$. In the TJ steady state the rates of these two processes must be equal each other, $R_+ = R_-$, so that we obtain $\theta_r = m\eta a_s \alpha(f)/fb$. It is easy to check that the function $\theta_r(f)$ has a minimum $\theta_r^* = \theta_r(f_m)$ at $f = f_m = 2T/a_s = T/\pi$, and the same is true for the $B(f)$ dependence: the normalized mobility first decreases and then increases with $f$ (note that the TJ state is stable with respect to fluctuations of $\theta_r$). Finally, the inequality $\theta_r(f) < \theta$ defines the range of model parameters and forces, where the TJ steady state could be stable, i.e., it should be $\eta < \eta_c \approx f e^{-\pi f/T}/2\pi\alpha_0 e^{-2/T}$.

This simple approach allows us to explain qualitatively the simulation results for the 1D FK-type models. The TJ state is stable for forces within the interval $f_{\rm b}' < f < f_{\rm forward}$, where $f_{\rm b}' > f_{\rm backward}$ because of $\theta_r < \theta$. To have the TJ state, the external damping $\eta$ due to the energy exchange with the substrate must be small, e.g., $\eta < 0.5$. In the elastic 1D FK model at a so small damping, the critical size of the TJ is very large: when an atom joins the TJ at its left-hand side, it excites a kink (local compression) in the TJ. This kink runs to the right-hand side of the TJ and stimulates the evaporation of the most right atom of the TJ. In the inelastic model, such an effect is absent (compare Figs. 2 and 7), the kink's motion is damped due to the intrinsic damping $\eta_l$. This explains a much wider range of model parameters, where the TJ state is stable in the soft FK model.

## 6. Conclusion

With the help of the numerical simulation, we have shown that the driven one-dimensional and two-dimensional FK models exhibit a hysteresis and the existence of traffic-jam states. First, the *hysteresis* does exist in the *underdamped* FK model for any *finite* rate of force changing. Secondly, *traffic jams* do appear in the *underdamped* FK model with *anharmonic* interaction. Already the hard-core potential, when the atoms do not interact at all except they cannot occupy the same well of the substrate potential, is sufficient to produce the traffic-jam behavior. Note that one might expect no transition to the traffic-jam state for the harmonic interatomic interaction. However, the situation is more subtle: there is no transition to the traffic-jam state for *atoms* in the standard 1D FK model, but the *kinks* may still be organized in jams because, for any short-ranged interatomic interaction, the interaction between the kinks is always exponential.

For the 1D FK model, the appearance of the inhomogeneous TJ state can be qualitatively explained with simple arguments as described in Sec. 5. Unfortunately, the behavior of the 2D FK model may be explained in the framework of a more simplified model only, e.g., such as the 2D two-state lattice-gas model [1].

Also we have shown that the dynamics of the soft model with inelastic interaction strongly differs from the classical (elastic) one. First, now the system exhibits a hysteresis even at high temperatures. The reason why the 1D model exhibits a hysteresis is that the soft model is effectively an infinite-dimensional one, the particles have an infinite number of internal degrees of freedom treated in a mean-field fashion. Secondly, the soft model allows the coexistence of two phases (the TJ state) for a much wider range of model parameters. Both these effects are due to the clustering of atoms in the soft model. The mechanism of clustering is analogous to that described in *et al* [11], although our model is essentially different: there is no artificial freezing in our model and, therefore, the correlated motion emerges solely due to the mutual damping of the NN atomic motion.

In the present work, we have shown the existence of the TJ state even in the 1D FK models with repulsive interaction, where the classical model cannot exhibit phase transitions. In a 2D or 3D system, especially if there is also an attractive branch of the interatomic interaction, the changes due to inelasticity should be even more dramatic. Of course, the damping mechanism cannot change the phase diagram of the system. But it certainly will change the kinetics of phase transitions as well as possible metastable states in which the system may be captured.

Finally, using the results of the present work, one can give a simple solution to how to avoid traffic jams: the particles (atoms in the FK model or cars in the one-lane road) should interact harmonically, i.e., they should try to keep an equidistant interval between themselves. Although this solution is quite trivial and has been well known empirically for a while, the simple models considered in the present paper allow us to study this question analytically.

This research was partially supported by the Ministry of Ukraine for Education and Science (Project No. F7/279-2001), the Hong Kong Research Grants Council (RGC) and the NATO Collaborative Linkage Grant PST.CGL.980044.

1. *Braun O.M., Hu B.*//Phys. Rev. E **71** (2005) 031111.
2. *Braun O.M., Kivshar Yu.S.* The Frenkel—Kontorova Model.— Springer, Berlin, 2004; Phys. Repts. 1998.— **306**.— P. 1.
3. *Bar'yakhtar V.G., Ivanov B.A., Sukstanskii A.L., Tartakovskaya E.V.*// Teor. Mat. Fiz.— 1988.— **74**.— P. 46.
4. *Baryakhtar I.V., Baryakhtar V.G., Economou E.N.*//Phys. Rev. E.— 1999.— **60**.— P.6645.
5. *Robbins M.O.*//Jamming and Rheology: Constrained Dynamics on Microscopic and Macroscopic Scales/Ed. by A.J. Liu and S.R. Nagel.— London: Taylor and Francis, 2000.
6. *Braun O.M., Hu B., Filippov A., Zeltser A.*//Phys. Rev. E.— 1998.— **58**.— P. 1311
7. *Movies* illustrating different regimes of the 2D FK model are available at http://www.iop.kiev.ua/∼obraun
8. *Tekic J., Braun O.M., Hu B.*// Phys. Rev. E.— 2005.— **71**.— P. 026104.
9. *Granular* Gases: Lectures Notes in Physics/Eds. T. Pöschel and S. Luding.— Berlin: Springer, 2001.— Vol. 564.
10. *Jaeger H.M., Nagel S.R., Behringer R.P.*//Rev. Mod. Phys.— **68**.— P. 1259.
11. *Cecconi F., Puglisi A., Marconi U.M.B., Vulpiani A.*//Phys. Rev. Lett.—2003.— **90**.— P. 064301.
12. *Braun O.M., Dauxois T., Paliy M.V., Peyrard M.*//Phys. Rev. E.— 1997.— **55**.— P. 3598.
13. *Braun O.M., Hu B.*// J. Stat. Phys.— 1998.— **92**.— P. 629.

## ФАЗОВА СЕГРЕГАЦІЯ В НЕЛІНІЙНИХ РУХОМИХ МОДЕЛЯХ

*О.М. Браун*

Р е з ю м е

Вивчається система ангармонійно взаємодіючих атомів в періодичному одновимірному і двовимірному зовнішньому потенціалі, що рухається завдяки зовнішній силі. Коли рушійна сила зростає, система переходить від нерухомого стану до стану ковзання, що відповідає рухомому кристалу. Показано, що перед переходом до стану ковзання система проходить через неоднорідний стан, в якому вона розщеплюється на області нерухомих атомів ("затори") і області рухомих атомів. Також запропонована нова модель, де частинки мають комплексну структуру, що трактується у наближенні середнього поля: зіткнення частинок є нееластичним, до того ж вважається, що кожна частинка володіє власним термостатом. Коли на атоми діє зовнішня сила, ця модель демонструє гістерезис і стан заторів реалізується для набагато ширшого діапазону параметрів моделі, ніж у класичній (еластичній) моделі, і обидва ці результати зберігаються при високих температурах.

## ФАЗОВАЯ СЕГРЕГАЦИЯ В НЕЛИНЕЙНЫХ ДВИЖУЩИХСЯ МОДЕЛЯХ

*О.М. Браун*

Р е з ю м е

Изучается система ангармонически взаимодействующих атомов в периодическом одномерном и двумерном внешнем потенциале, которая движется под действием внешней силы. Когда движущая сила возрастает, система переходит от неподвижного состояния к состоянию скольжения, соответствующему движущемуся кристаллу. Показано, что перед переходом к состоянию скольжения система проходит через неоднородное состояние, в котором система расщепляется на области неподвижных атомов ("автомобильные пробки") и обла-

сти бегущих атомов. Также предложена новая модель, где частицы имеют сложную структуру, рассматриваемую в приближении среднего поля: столкновения частиц считаются неэластичными, а каждая частица считается обладающей собственным термостатом. Когда внешняя сила приложена к атомам, эта модель демонстрирует гистерезис и режим автомобильных пробок для намного более широкого диапазона параметров модели, чем классическая (упругая) модель, причем оба эти результата наблюдаются и при высоких температурах.