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Phase segregation in driven diffusive systems

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Abstract

Driven diffusive models describe an array of atoms in an external periodic potential, when the motion is damped due to energy exchange with the substrate. The systems of this class have wide application in modeling of charge and mass transport in solids. Recently, the driven diffusive models have been used in tribology, where the driving force emerges due to motion of one of two substrates, which are separated by a thin atomic layer. When a dc force is applied to the atoms, the system exhibits the locked-to-sliding transition. During the transition the system may split in domains of two kinds, the running domains where the atoms move with almost maximum velocity, and the immobile domains ("traffic jams"). We discuss a new model for a 1D chain, where the particles have a complex structure treated in a mean-field fashion: particle collisions are inelastic and also each particle is considered as having its own thermostat. This model exhibits a hysteresis and the "traffic jams" state even at high temperatures due to the clustering of atoms with the same velocity.

Keywords: Driven system; Hysteresis; Jamming

1. Introduction

Driven diffusive systems belong to 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 modeling of charge and mass transport in solids. Last years

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the driven diffusive models are used in tribology, where the driving force emerges owing to motion of one of two substrates separated by a thin atomic layer.

We consider phase segregation in a system consisting of complex particles which have their own structure with internal degrees of freedom. The internal modes may be excited due to inter-particle collisions that take away the kinetic energy of the translational motion so that the collisions are inelastic. This is a typical situation in soft-matter physics, e.g., in physics of granular gases [1–3].

The kinetic energy of atomic translational motion that is lost in a collision is stored as the energy of excitation of internal degrees of freedom and may be released later as 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 in collisions is transformed into the "heating" of particles. We propose a new type of stochastic models, the model with "multiple" thermostats, where, in addition to the standard "substrate" thermostat, each particle is considered as having its own "thermostat". A natural description of such a model is one with a specific type of Langevin equations.

2. Model

Let us consider a one-dimensional (1D) system of particles with nearest-neighbors (NN) inelastic interaction, subjected to a sinusoidal substrate potential $V_{\rm sub}(x) = \frac{1}{2}\varepsilon_s[1 - \cos(2\pi x/a_s)]$. It is a generalization of the well-known Frenkel–Kontorova (FK) model (e.g., see [4] and references therein). Namely, we consider a chain of N atoms distributed over M minima of the substrate potential with periodic boundary conditions. The equation of motion for the lth particle has the form

$$m\ddot{x}_l + m\eta\dot{x}_l + V'_{\rm sub}(x_l) = -f_{l+1,l} + f_{l,l-1} + \delta F_l(t) + f\,, \tag{1}$$

where the dot (prime) indicates the time (spatial) derivative. To each atom we apply an external dc force f and a viscous damping force. The coefficient η describes the energy exchange with the substrate. The substrate thermostat is modeled by the Gaussian stochastic force, $\delta F_l(t)$, which has zero average and the standard correlation function

$$\langle \delta F_l(t)\delta F_{l'}(t')\rangle = 2\eta m k_B T \delta_{ll'}\delta(t - t')\,, \tag{2}$$

where T is the temperature and k_B is Boltzmann's constant. Throughout the paper we use dimensionless units with $m = 1$, $a_s = 2\pi$ and $\varepsilon_s = 2$. Also, we set $k_B = 1$, so that T is measured in energy units.

The interaction is chosen in an exponential form, $V_{\rm int}(x) = V_0\exp(-\gamma x)$. The amplitude, V_0, is related to the effective elastic constant g, $g = (a_s^2/2\pi^2\varepsilon_s)V''(a_A)$, where $a_A = a_s M/N$ is the average distance between the atoms. The exponential potential reduces to the harmonic one in the limit $\gamma \to 0$ and to the hard-core potential in the limit $\gamma \to \infty$.

The inelasticity of collisions is modeled by a viscous damping force proportional to the relative velocity of two atoms. The mutual interaction between the lth and

$(l-1)$th atoms is described by the force $f_{l,l-1}$:

$$f_{l,l-1} = -V'_{\rm int}(x_l - x_{l-1}) - m_r\eta_l(\dot{x}_l - \dot{x}_{l-1}) + \delta f_l(t)\,. \tag{3}$$

The first term on the r.h.s. of Eq. (3) describes the elastic interaction, the second term describes the inelasticity due to viscous damping, $m_r = m/2$ is the reduced mass of two colliding atoms, and the last term is the stochastic force that compensates the energy losses due to inelasticity,

$$\langle \delta f_l(t)\delta f_{l'}(t')\rangle = 2\eta_l m_r k_B T\delta_{ll'}\delta(t-t')\,. \tag{4}$$

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

The set of Langevin equations (1)–(4) is equivalent to the Fokker–Planck–Kramers equation for the distribution function $W(\{x_l\},\{\dot{x}_l\};t)$,

$$\begin{aligned}\frac{\partial W}{\partial t} + \sum_l \left\{ \dot{x}_l \frac{\partial W}{\partial x_l} + [f - V'_{\rm sub}(x_l) + V'_{\rm int}(x_{l+1} - x_l) - V'_{\rm int}(x_l - x_{l-1})]\,\frac{\partial W}{\partial \dot{x}_l}\right\} \\ = \frac{1}{2}\sum_l \frac{\partial}{\partial \dot{x}_l}\left[(2\eta + \eta_{l+1} + \eta_l)\left(\dot{x}_l + T\frac{\partial}{\partial \dot{x}_l}\right)\right. \\ \left. - \eta_{l+1}\left(\dot{x}_{l+1} + T\frac{\partial}{\partial \dot{x}_{l+1}}\right) - \eta_l\left(\dot{x}_{l-1} + T\frac{\partial}{\partial \dot{x}_{l-1}}\right)\right] W\,.\end{aligned} \tag{5}$$

It is easy to check that in the undriven case, $f = 0$, the Maxwell–Boltzmann distribution is a solution of Eq. (5). Thus, the inelastic FK model introduced above, has the truly thermodynamically equilibrium state.

In the driven case, $f \neq 0$, the thermal equilibrium state is destroyed and the system exhibits a transition from a 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, when the interactions are elastic, the locked-to-sliding transition was studied in a series of papers [5–7]. At zero temperature, $T = 0$, the average velocity of the atoms as a function of f exhibits hysteresis, but at any $T > 0$ the hysteresis disappears for an adiabatically slow change of the driving in the 1D model. Besides, for nonlinear interactions, the steady state during the locked-to-sliding transition for some range of model parameters may correspond to a specific ''traffic-jam'' (TJ) state with an inhomogeneous spacial distribution of atoms [5,6].

In the present work, we show that both of these properties of the transition change drastically for an inelastic interaction. First, the system exhibits hysteresis even at very high temperatures. Second, the TJ regime is observed for a much wider range of model parameters, thus, it is a generic property of the system. Both effects appear because of a clustering of atoms as was predicted by Cecconi et al. [3]. Indeed, in the case of inelastic interaction, the energy losses are minimal when the NN atoms move with the same velocity and the mutual viscous forces are zero.

3. Results

In simulations, we choose $N/M = \frac{144}{233}$, which is close to the "golden-mean" atomic concentration. The force was typically changed at the rate $R \equiv \Delta f/\Delta t \approx 2 \times 10^{-7}$, which is low enough to be considered as adiabatically slow. Typically, we used the following parameters: $\eta = 0.01$, $\gamma = 1/\pi$ so that the dimensionless anharmonicity parameter is $\gamma a_s = 2$, $g = 1$ (recall that in the classical FK model the Aubry locked-to-sliding transition [8] takes place with the increase of g at $g \approx 1$), and $T = 1$ which is quite large as compared with the barrier height $\varepsilon_s = 2$.

The simulation results for the normalized mobility $B = \langle v \rangle / v_f$ are presented in Fig. 1. Here, $\langle v \rangle = \sum_{l=1}^{N} \langle \dot{x}_l \rangle_t / N$, $\langle \ldots \rangle_t$ stands for averaging over time and $v_f \equiv f/m\eta$ is the maximum atomic velocity. One can see that while there is no hysteresis in the $B(f)$ dependence in the "elastic" model (a narrow hysteresis of the width $\Delta f = 0.0025$ exists due to the finite step of force changing), hysteresis does exist for $\eta^* > 0$ and its width strongly increases with η^*. Moreover, the width of the hysteresis does not change essentially if the rate of force variation changes in 25 times as shown in the inset in Fig. 1 (left panel). We emphasize that the hysteresis in Fig. 1 is for a quite large temperature $T = 1$, and it survives even at $T = 2$, when $\varepsilon_s/k_B T = 1$. In the case $\eta^* \approx 0.0393$, the dependence $\Delta F(T) = f_{forward}(T) - f_{backward}(T)$ 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 $\Delta F(T) \lesssim \Delta f$ which gives $T_m \gtrsim 3.15$.

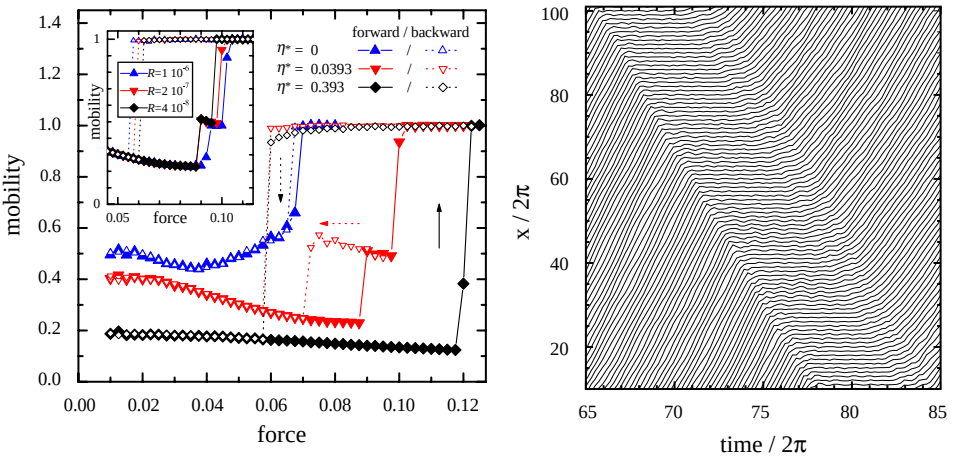

Fig. 1. Left panel: dependence of the normalized mobility B on the force f for three values of the intrinsic damping: $\eta^* = 0$ (up triangles, the "elastic" model), $\eta^* = e^{-a_A} \approx 0.0393$ (down triangles), and $\eta^* = 10\,e^{-a_A} \approx 0.393$ (diamonds) for an increasing force (solid curves and symbols) and a decreasing force (dotted curves and open symbols). Other parameters are the following: $\gamma = 1/\pi$, $g = 1$, $\eta = 0.01$, 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), $R \approx 2 \times 10^{-7}$ (down triangles), and $R \approx 4 \times 10^{-8}$ (diamonds). Right panel: atomic coordinates as functions of time in the "traffic-jam" regime for $f = 0.095$, $\eta^* \approx 0.0393$, $\gamma = 1/\pi$, $g = 1$, $\eta = 0.01$, and $T = 1$.

Qualitatively the existence of hysteresis may be explained in the same way as in Ref. [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 expand over the whole system. In the "soft" model considered here, where a fluctuation of the relative velocity of the NN atoms is suppressed, the probability of the emergence of a nucleus with a maximum velocity in 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 FK model. One more indication of this effect is the plateau at $B\sim 0.5$ in the $B(f)$ dependence of Fig. 1, which corresponds to the TJ regime. The TJ state appears in the interval of forces $0.09 \leqslant f \leqslant 0.0975$ in the force-increasing process and survives till $f \geqslant 0.0725$ if the force decreases starting from the TJ state. The atomic trajectories in the TJ state are shown in Fig. 1 (right panel). In Refs. [5,6] we have shown that in the anharmonic FK model the inhomogeneous state may correspond to the TJ state when the chain splits into regions of totally immobile atoms (TJ) separated by regions of running atoms. The same TJ state appears in the present model and, moreover, now it is observed for a much wider range of model parameters and high temperatures.

The phase segregation in the driven model can be explained with the help of the generalized lattice-gas model [9]. As was shown in Refs. [5,6,9], the normalized mobility of the steady state with a coexistence of two phases, the TJ phase consisting of locked atoms and the running domain (RD), is equal to $B = b\theta_r(1-\theta)/(1-\theta_r)\theta$, where $b = v_r/v_f \approx 1$, $\theta = N/M$, θ_r is the local concentration in the RD and v_r is the average atomic velocity in the RD (see Fig. 1, right panel). In the case of a single TJ in the sea of running atoms, TJ grows from its left-hand side with the rate $R_+ = v_r/a_r$, where $a_r = a_s/\theta_r$, while from its right-hand side TJ shortens with a rate R_- due to "evaporation" of the right-most atom of TJ into RD. At a low temperature and driving force, when $\varepsilon(f) \approx \varepsilon_s - fa_s/2 \gg T$, the "evaporation" of the right-most atom of TJ is an activated process and its rate is $R_-(f) \propto \exp[-\varepsilon(f)/T]$. The TJ may exist only if $R_- \leqslant \max R_+$. This leads to a condition on the temperature, i.e., T must be lower than some critical value. In the TJ steady state the growing and evaporating rates must be equal to each other, $R_+ = R_-$. This gives $\theta_r = m\eta a_s R_-(f)/fb$. The function $\theta_r(f)$ has a minimum at $f = 2T/a_s$, and the same must be true for the $B(f)$ dependence: the normalized mobility first decreases and then increases with f. This is in agreement with the simulation results of Fig. 1. The inequality $\theta_r(f) < \theta$ defines the range of model parameters and forces, where the TJ steady state could be stable, i.e., the damping η should be lower than some critical value $\eta' \sim 0.5$.

4. Conclusion

Thus, the TJ state may appear only in the underdamped system when the substrate damping η is low enough and an atom exhibits bistability, i.e., when both states, the

locked state and the running state, coexist (and are dynamically stable) at the same driving f. Then the locked-to-running transition should always pass through the TJ state. In the soft model with inelastic interaction, the system exhibits hysteresis even at high temperatures. The reason why the 1D model exhibits hysteresis is that the soft model is effectively infinite-dimensional. The particles have an infinite number of internal degrees of freedom treated in a mean-field fashion. Second, the soft model allows the coexistence of two phases (the TJ regime) for a much wider range of model parameters. Both effects are due to the clustering of atoms in the soft model. The mechanism of clustering is the same as described by Cecconi et al. [3], but our model is essentially different from the latter. There is no artificial freezing in our model and, as a result, the correlated motion emerges solely due to the mutual damping of the NN atoms.

In the present work, we considered the 1D model with a repulsive interaction, when the classical (elastic) model should not 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.

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