Clustering of atoms in a model with multiple thermostats

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We propose a model for a one-dimensional chain of interacting particles in an external periodic potential. In this model 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. We derived the Fokker-Planck equation for this model and demonstrated that the model has a truly equilibrium ground state. When an external dc force is applied to the atoms, the model exhibits a hysteresis even at high temperatures due to the clustering of atoms with the same velocity. Another effect of clustering is phase separation in the steady state when the system splits into regions of immobile atoms ("traffic jams") and regions of running atoms.

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We consider the problem of modeling 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 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, for example, in physics of granular gases [1,2]. A direct simulation of such a system that takes into account a detailed internal structure of particles is too time consuming, hence alternative simplified models are of interest.

Recently Cecconi *et al.* [3] have studied a model of such type. In their model there are two "atoms" in the double-well external potential and the atomic collisions are inelastic (the authors considered the simplest case of hard-core collisions). The model exhibits an interesting effect of atom "clustering," when both atoms prefer to stay in the same well of the substrate potential and, moreover, at low temperatures both atoms hop simultaneously over the barrier that separates the wells. The model of Cecconi *et al.* [3], however, violates the energy conservation principle: the energy that is lost in collisions disappears forever. As a result, a stationary state of such a model does not correspond to a thermally equilibrium state; the energy losses due to collisions lead to an effective cooling of the system. In the context of granular matter physics, where grains are typically macroscopic particles, the violation of energy conservation is irrelevant, because energy losses are negligible with respect to other energies involved in the problem [1–5]. But for mesoscopic or microscopic particles (e.g., macromolecules) the energy losses in inelastic collisions may be essential.

In a more realistic physical model 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. In the present work we propose a different type of stochastic models, a 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 (or the corresponding Fokker-Planck equation). Although the atomic interactions are inelastic, the model does have a truly thermally equilibrium state with a Maxwell-Boltzmann distribution so long as there are no external forces.

As a typical example, we consider an infinite one-dimensional (1D) system of "atoms" with nearest-neighbors (NN) inelastic interaction, subjected to a sinusoidal substrate potential. It is a generalization of the well-known Frenkel-Kontorova (FK) model (e.g., see Ref. [6] and references therein). We consider a chain of N atoms distributed over M minima of the sinusoidal substrate potential $V_{\mathrm{sub}}(x)=\frac{1}{2}\varepsilon_s[1-\cos(2\pi x/a_s)]$ with periodic boundary conditions. The equation of motion for the lth particle has the form

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

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

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

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.

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The interaction takes an exponential form, $V_{\rm int}(x) = V_0 \exp(-\gamma x)$. The amplitude V_0 is related to the effective elastic constant g, $g=(a_s^2/2\pi^2\varepsilon_s)V''(a_A)=V_0\gamma^2\exp(-\gamma a_A)$, and $a_A=a_sM/N$ 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 $f_{l,l-1}$:

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

The first term on the right-hand side 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 loss due to inelasticity,

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

The mutual damping η_l was 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 $W(\{x_l\},\{\dot{x}_l\};t)$,

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

It is easy to check that in the undriven case, $f=0$, the Maxwell-Boltzmann distribution is a solution of Eq. (5). Thus our model 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 [7–9]. 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. However, in actual simulation when the force f changes at a finite rate, a small hysteresis persists due to the delay in forming the steady state. Besides, in the case of exponential 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 [7,8].

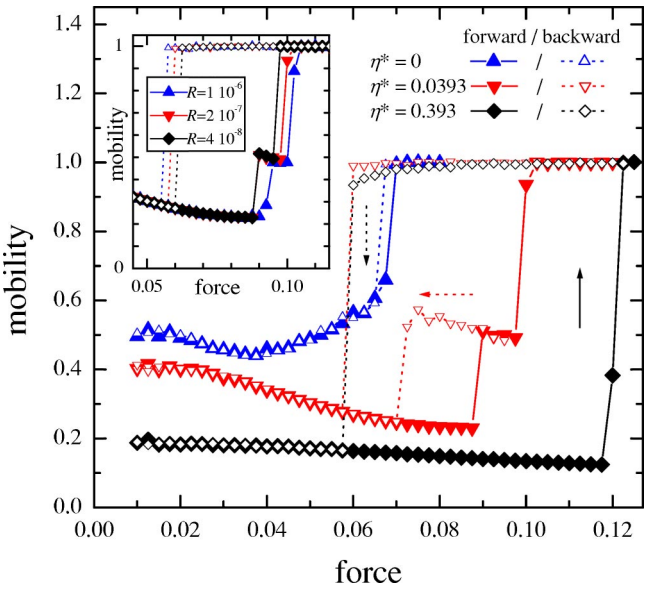

FIG. 1. (Color online) Dependence of the normalized mobility B on the force f for three values of the intrinsic damping: $\eta^*=0$ (blue up triangles, the elastic model), $\eta^*=e^{-a_A}\approx 0.0393$ (red down triangles), and $\eta^*=10e^{-a_A}\approx 0.393$ (black diamonds) for an increasing force (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: $R\approx 10^{-6}$ (blue up triangles), $R\approx 2\times 10^{-7}$ (red down triangles), and $R\approx 4\times 10^{-8}$ (black diamonds).

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.

In simulations, we choose $N/M=144/233$, which is close to the "golden-mean" atomic concentration. The force was typically changed at the rate $R\equiv\Delta f/\Delta t=0.0025/(2\times 1000\times 2\pi)\approx 2\times 10^{-7}$, 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 [10,11] 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 $\langle v\rangle=\Sigma_{l=1}^N\langle\dot{x}_l\rangle_t/N$, $\langle\cdots\rangle_t$ stands for averaging over time and $v_f\equiv f/m\eta$ is the maxi-

mum 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. We emphasize that the hysteresis in Fig. 1 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 $\Delta F(T)\lesssim\Delta f$ which gives $T_m\gtrsim 3.15$.

Another important parameter of the model under consideration is the rate of energy exchange with the substrate. When the damping η increases, the width of the hysteretic loop decreases and the system behavior approaches that of the elastic model. For example, for $\eta^*\approx 0.0393$ and $T=1$ the hysteresis disappears at $\eta\gtrsim\eta^*$. When the other two parameters of the model, i.e., the strength of interaction g and the radius of interaction γ are varied, the system behavior remains qualitatively the same as described above.

Qualitatively the existence of hysteresis may be explained in the same way as in Ref. [8]. 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 traffic-jam regime. The TJ state appears in the interval of forces $0.09\leqslant f\leqslant 0.0975$ in the force-increasing process and survives until $f\geqslant 0.0725$ if the force decreases starting from the TJ state. The atomic trajectories in the TJ state are shown in Fig. 2. An inhomogeneous metastable state in the driven classical FK model was found by Strunz and Elmer [12]. In Refs. [7,8] 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 (traffic jams) 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.

To study the TJ state, we calculated the coordinate and velocity correlation functions of the NN atoms, $K_x=\langle(x_l-x_{l-1}-a_A)^2\rangle$ and $K_v=\langle(\dot{x}_l-\dot{x}_{l-1})^2\rangle$, where $\langle\cdots\rangle$ stands for the spatial average along the chain as well as the temporal average over the time interval $\Delta t=2000\pi$. For a spatially homogeneous state we should have $K_x\approx K_{x0}=T/g$ and $K_v\approx K_{v0}=2T$, whenever for an inhomogeneous (TJ) state much higher values are expected. Indeed, the dependencies presented in Fig. 3 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. 1, the TJ state disappears at low damping ($\eta^*=0$) as well as at very high values of η^* (e.g., $\eta^*=0.393$).

As was shown in Refs. [7,8,13], 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. 2). In the case of a single TJ in the sea of running atoms, TJ grows

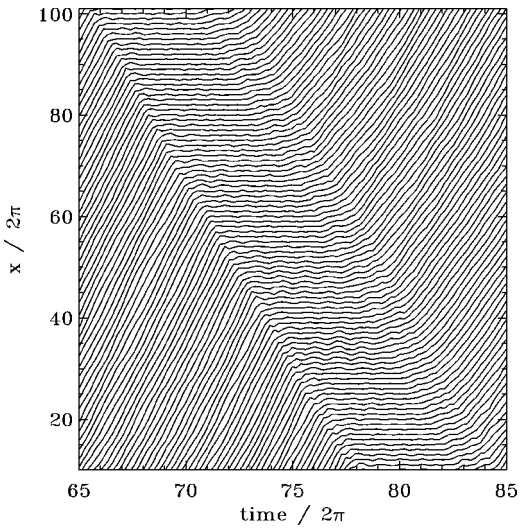

FIG. 2. Atomic coordinates as functions of time in the traffic-jam regime for $f=0.095$, $\eta^*\approx 0.0393$, $\gamma=1/\pi$, $g=1$, $\eta=0.01$, and $T=1$.

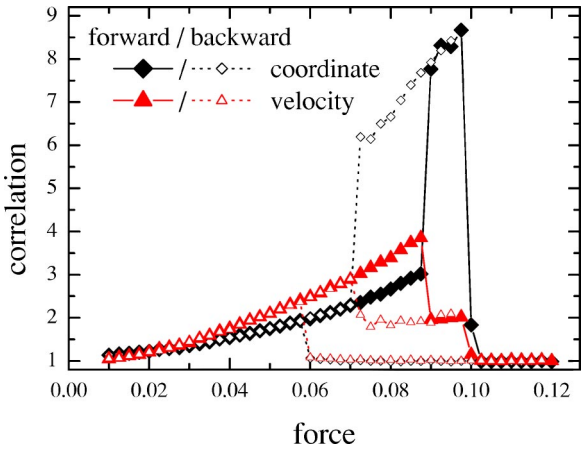

FIG. 3. (Color online) Dependence of the normalized correlation of coordinates K_x/K_{x0} (black diamonds) and velocities K_v/K_{v0} (red triangles) on the driving force f for $\eta^*\approx 0.0393$, $\gamma=1/\pi$, $g=1$, $\eta=0.01$, and $T=1$ for an increasing force (solid curves and symbols) and a decreasing force (dotted curves and open symbols).

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 $\eta' \sim 0.5$.

This simple approach allows us to explain the simulation results. 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, and the only question is about the stability of this TJ state. In the elastic FK model at a small damping η the critical size of the TJ is very large. When an atom joins the TJ on its left-hand side, it excites a kink (local compression) in the TJ. It then runs to the right-hand side of the TJ and stimulates the evaporation of the right-most atom of the TJ [8]. In the inelastic model this effect is absent. The kink motion is damped due to intrinsic damping η_i; therefore the TJ regime is much more stable.

Thus we have shown that the dynamics of the soft model with inelastic interaction drastically differs from the classical (elastic) one. First, 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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