Dynamic rigidity transition

J. A. Åström,[1,2] M. Latva-Kokko,[1] and J. Timonen[1]
[1]*Department of Physics, University of Jyväskylä, P.O. Box 35, FIN-40351 Jyväskylä, Finland*
[2]*Laboratory of Physics, Helsinki University of Technology, P.O. Box 1100, FIN-02015 Helsinki, Finland*
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An inflated closed loop (or membrane) is used to demonstrate a dynamic rigidity transition that occurs when impact energy is added to the loop in static equilibrium at zero temperature. The only relevant parameter in this transition is the ratio of the energy needed to collapse the loop and the impact energy. When this ratio is below a threshold value close to unity, the loop collapses into a high-entropy floppy state, and it does not return to the rigid state unless the impact energy can escape. The internal oscillations are in the floppy state dominated by $1/f^2$ noise. When the ratio is above the threshold, the loop does not collapse, and the internal oscillations resulting from the impact are dominated by the eigenfrequencies of the stretched membrane. In this state, the loop can bounce for a long time. It is still an open question whether bouncing will eventually vanish or whether a stationary bouncing state will be reached. The dynamic transition between the floppy and the rigid state is discontinuous.

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I. INTRODUCTION

Rigidity transitions have attracted a lot of interest during recent years [1]. The rigidity of a connected network is governed by the amount of elastic constraints in relation to the number of degrees of freedom. The distribution of the constraints is also important as the overconstraining of some degrees of freedom does not add to rigidity. A square lattice in a two-dimensional space with sites connected through central-force potentials is right at the rigidity threshold. The number of floppy modes per degrees of freedom can be written as [2] $f=1-\langle z\rangle/z^*+n_r$, where $\langle z\rangle$ is the number of constraints per node, $z^*=4$ is the number of constraints at the rigidity threshold, and n_r is the number of redundant bonds per degree of freedom. There are obviously no redundant bonds in a square lattice, and $\langle z\rangle=4$. The lattice can nevertheless be sheared without any elastic resistance. However, adding one single constraint anywhere in the lattice in the form of a diagonal spring will make it rigid (if periodic boundary conditions are imposed [3]). Replacing the central-force springs with vector-potential beams (which have both bending and tensile stiffness) would take the square lattice far above (i.e., in terms of constraints) the rigidity threshold. On the other hand, a central-force network with the structure of a random network of fibers is not rigid at any finite density of fibers, but can be driven through a rigidity transition by adding extra constraints [6,4,5]. In these models, rigidity thus appears as a result of increasing the number of constraints to a formerly flexible structure.

Constraint-counting methods can only give the zero-temperature equilibrium of the system. At nonzero temperatures the equilibrium must be determined through an appropriate free energy. For a system in a heat bath, e.g., the equilibrium is given by the minimum of the Helmholtz free energy $F=E-TS$, in which entropy plays an important role as soon as $T>0$. If a system does not have floppy modes, its mechanical equilibrium is typically governed by internal energy, and entropy can be neglected. Floppy motions do not cost internal energy, but they do cost [7] free energy. For $T>0$ there are thus stochastic restoring forces of entropic origin, as has been demonstrated [7] for randomly diluted lattices. Close to the rigidity percolation threshold, and in some cases below it, the entropic contributions to rigidity dominate at any $T>0$. In diluted central-force lattices, entropic rigidity appears above the connectivity-percolation threshold, which typically is different [2–4] from the rigidity-percolation threshold.

In this paper we investigate in terms of rigidity the dynamics of a simple structure when the ratio of the bending to tensile stiffness is variable. For this purpose we use a simple model for a closed membrane, a one-dimensional closed loop of mass points connected by springs. For this structure, $\langle z\rangle=2$, which means that it is clearly below the rigidity threshold. If, however, the loop is stretched it will become rigid. A natural way to stretch a one-dimensional closed loop in a two-dimensional space is to ''inflate'' it. The stiffness of a local bending of the membrane will then become $\epsilon\tau/2$, where ϵ is the spring constant and τ is the tension caused by the inflation pressure. This takes the loop right to the rigidity threshold, and the number of floppy modes vanishes. A straightforward way of understanding this is to describe the internal pressure such that it forces the mass points to be at a fixed distance from the center of the loop. This adds N constraints, if N is the number of mass points. The coordination of each of the mass points in the spring loop is increased by 1, and the coordination of the center point is N. The average coordination of the system is hence increased by $1+(N-3)/(N+1)\to 2$ as $N\to\infty$. This system is somewhat above the rigidity threshold. It can be used to study the rigidity transition by increasing temperature, or by imposing on it a mechanical disturbance, which will induce a dynamic transition to a flexible state. This will make some of the constraints marginal and transform a formerly rigid structure into a flexible one. We apply this method below.

II. NUMERICAL MODEL

A minimal model for a membrane is given by a closed loop of mass points connected by linear elastic springs (a

minimal model also for a polymer loop). The equations of motion for this model can be written in the form

$$m\ddot{\vec{\mu}}_i = \tau_i \vec{\eta}_i - \tau_{i+1}\vec{\eta}_{i+1} + P(l_0/2)\vec{\nu}_i + P(l_0/2)\vec{\nu}_{i+1}, \quad (1)$$

where m are the masses at points $\vec{\mu}_i$ connected by springs with tension forces τ_i, P is the inflating pressure, l_0 is the equilibrium length of the springs, $\vec{\eta}_i$ is a unit vector along spring i, and $\vec{\nu}_i$ is the outward unit normal to the same spring. To further simplify the model, we assume that pressure P is independent of the area inside the loop (i.e., like osmotic pressure).

This numerical model is rather similar to the ones used to describe biological membranes [8]. The main difference between the two cases is that, in our case, inertia plays a significant role in the properties of the system.

We demonstrate below that, when τ becomes very small, even a minor disturbance of the loop will then make it behave like a nonrigid structure (e.g., by inducing a mechanical deformation or raising the temperature slightly above zero). As τ increases, this disturbance has to be larger for flexible behavior to appear. In the case of mechanical deformation, the induced rigidity transition involves dynamics of the system.

An obvious way to study the dynamics of a two-dimensional inflated loop is to let it bounce. Bouncing of an inflated loop may seem a rather trivial problem as we are used to think of cases in which energy dissipation is strong. But what happens if dissipation is weak and inflation pressure is lowered until rigidity begins to vanish? And what will happen to rigidity at higher pressures when the center-of-mass (c.m.) kinetic and potential energies of the loop begin to transform into internal oscillations (i.e., oscillations of the mass points relative to the center of mass)?

We first relax the loop to a static equilibrium and then drop it through empty space onto a nondissipative elastic substrate (i.e., there is a repulsive linear elastic force preventing the mass points from penetrating deep into the substrate, but there is no inertia related to the deformation of the substrate and, therefore, all energy is returned to the loop). There is thus no mechanism for dissipating the energy that is initially stored in the form of potential energy in the gravitational field, and the work done by the inflation pressure, stored as an elastic tension of the membrane. Snapshots of simulations on this system are shown in Fig. 1.

III. RESULTS

As described above, we consider now a loop that is let drop freely from a fixed height above a substrate. At high inflation pressures, the behavior of the loop is very much as expected: regular bouncing with eigenfrequency oscillations in the membrane resulting from the impacts [Fig. 1(a)]. Bouncing is not regular, however. The loop bounces chaotically and the energy is slowly turned into internal oscillations. From the simulation results alone it is not possible, however, to reach a conclusion whether some bouncing will continue forever or if it will eventually cease. As anticipated

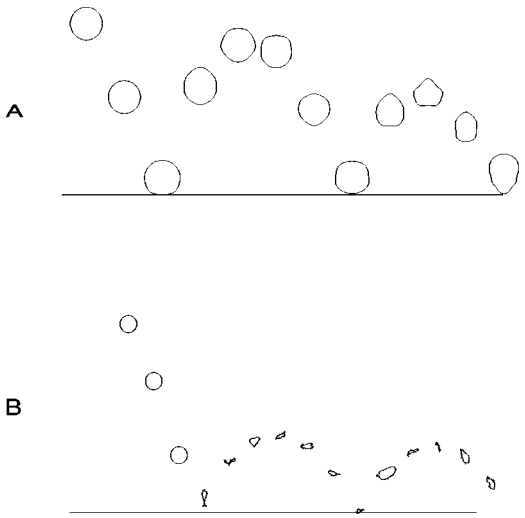

FIG. 1. Snapshots of bouncing closed membranes. (a) $\kappa = 3.7$ and (b) $\kappa = 0.5$.

above, a transition in the behavior of the loop takes place when the inflation pressure is lowered below a threshold. This transition first occurs close to the point where the potential energy equals the energy needed to fully collapse the loop. For pressures below the threshold, the loop collapses at the first bounce, and it never regains its shape [Fig. 1(b)]. When the two energies are almost equal, there is a kind of resonance, which means that bouncing vanishes very rapidly (after only a few bounces). This situation is shown in Fig. 2. The collapsed state bears all the trademarks of a flexible structure, while the uncollapsed state behaves as a rigid structure. In this sense the transition (collapse at the first impact) is a rigidity transition. The transition differs however from the ''ordinary'' rigidity transitions, in that it occurs only as a result of adding energy and not as a result of manipulating the number of constraints. We call it therefore a dynamic rigidity transition.

We analyze the situation in several different ways. First we analyze the equilibrium size of a closed loop in thermal equilibrium with a heat bath. The loop has a high-entropy collapsed state for radii below the zero-pressure static equilibrium radius. This state will be preferred at low pressures and high temperatures. At low temperatures and high pressures, the loop will be in a low-entropy uncollapsed state.

The numerical results for the bouncing loop begin with the Fourier spectrum for its internal oscillations. If the loop is flexible, the Fourier spectrum of the oscillations of the loop will be dominated by zero-frequency modes. If the loop is rigid, the oscillations are dominated by eigenfrequencies of the membrane. Collapse to a highly deformed ''flat'' state is then analyzed by following the height of the first bounce and the number of mass points that touch the substrate when

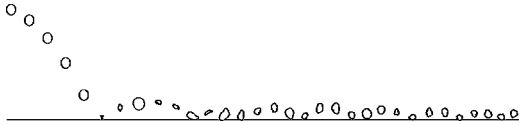

FIG. 2. Snapshots of a bouncing closed membrane at resonance.

the loop bounces. The loop radius is determined in the rigid as well as in the collapsed state, and the simulation results are compared against the theoretical results for a loop in thermal equilibrium. In the collapsed state, this means a suitable ''temperature'' is assigned to the loop. This impact-induced temperature is also compared with the thermodynamic transition temperature.

Finally we analyze the bouncing height of a rigid loop as a function of time. We demonstrate that, at high pressures, there is initially a rather fast decreasing trend in the bouncing heights, which later slows down considerably. We cannot judge whether all of the energy will turn into internal oscillations and if bouncing will eventually cease, or if a steady state will be reached. At later times, the differences in the bouncing heights are dominated by more or less stochastic fluctuations.

A. Free energy of a loop in thermal equilibrium

We first consider a loop such as that described above, in thermal equilibrium with a heat bath at temperature T. Its free energy F, as a function of the average radius r and temperature, can be approximated by

$$F = U(r_0 - r)\frac{3kT(2\pi)^2}{2Nl_0^2}(r^2 - r_0^2) + NPl_0(r_0 - r) + U(r - r_0)N\epsilon l_0 r_0 \sin(\pi/N)\left(\frac{r - r_0}{r_0}\right)^2, \tag{2}$$

where $r_0 \equiv (2\pi)^{-1}Nl_0$, ϵ is the spring constant, k is the Boltzmann constant, and U is the Heaviside unit step function. The first term on the right hand side arises from the entropy of a loop of circumference Nl_0, and of end-to-end distance $2\pi r$ [9]. The ''free distance'' of the loop between its end points is here assumed to describe a random walk. In a stretched loop ($r > r_0$) the end-to-end distance is fixed, and its entropy vanishes. The second term on the right hand side is work against the inflation pressure, and the third term is the radial component of the elastic energy of the membrane springs. Minimizing F with respect to r gives

$$r = \frac{Pr_0}{2\epsilon \sin(\pi/N)} + r_0 \tag{3}$$

for $r > r_0$, and

$$r = \frac{N^2 l_0^3 P}{12\pi^2 kT} \tag{4}$$

for $r < r_0$.

We estimate the transition point T_c by equalling the free energy Eq. (2) for the two possible states of the loop, and find that

$$kT_c = \frac{1}{3}\frac{(Pr_0)^2}{\epsilon} \tag{5}$$

when N is assumed to be large. For large T and small P, $r < r_0$, and for small T and large P, $r > r_0$. The transition is discontinuous. In the rigid state ($r > r_0$) the system is that of coupled oscillators, and the average loop radius is given by the energy minimum (vanishing entropy) of the system, while in the flexible state ($r < r_0$) there are entropic restoring forces [7], and the loop radius is fluctuating, with an average value given by the free-energy minimum. Notice, however, that in this case the restoring forces appear only as a result of the changes in the average radius of the loop, and the structure is therefore flexible.

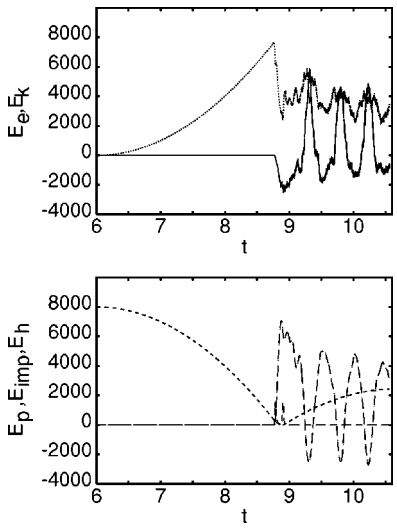

FIG. 3. The energy components of the system as a function of time. (a) The kinetic energy increases until the loop hits the substrate, whereafter it drops and then oscillates with a small amplitude. The elastic energy decreses at the first impact and begins then to oscillate. (b) The potential energy describes the bouncing motion of the loop. The impact energy is nonzero only when the loop is in contact with the substrate. The work against the inflation pressure oscillates roughly out of phase with the elastic energy oscillation.

B. Fourier spectrum of the internal oscillations

We now return to the model of a closed loop that is let drop from height h_0 above a substrate, and which then bounces off that substrate. The energy of the bouncing loop has five different components: The elastic energy (E_e) of the springs, the kinetic energy of the mass points (E_k), the potential energy in the gravitational field (E_h), the elastic energy of deformation of the substrate during impacts (E_{imp}), and the work done against the pressure as the loop is deformed (E_p). Figure 3 shows these energy components for a single simulation. First, when the loop is being dropped, potential energy is transformed into kinetic energy, while all the other components vanish. When the loop bounces the first time, there will be a complicated exchange of energy between the different components. The evolution of the subsequent bouncing heights will thus become highly nontrivial.

We benchmarked the model we use by recording all energy components during the simulations. The total energy of the system was found to vary by less than $\pm 0.01\%$, which we found very satisfactory.

Fourier spectra of the internal oscillations of the loop can be used to characterize their properties, and some of them are

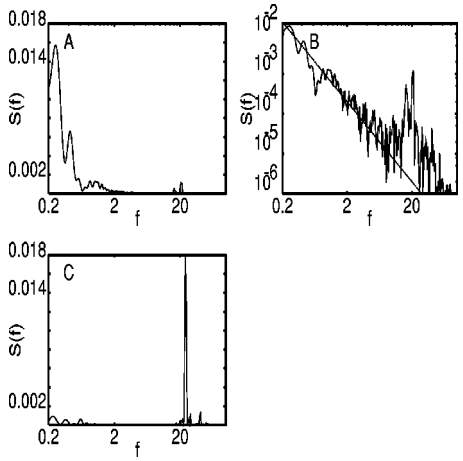

FIG. 4. Fourier spectrum of the motion of the mass points with respect to the center of mass of the membrane, calculated over a few bounces. (a) $Pl_0=e^1$ on a linear scale. (b) $Pl_0=e^1$ on a logarithmic scale. The low frequency modes are compared to $1/f^2$. (c) $Pl_0=e^5$. The dominant frequency is located at $f=21$, which is approximately equal to the eigenfrequency corresponding to $n=2$, $f_n=23.2$.

shown in Fig. 4. At a low pressure [Figs. 4(a) and 4(b), $Pl_0=e^1$] these oscillations seem to be dominated by Brownian (thermal) motion of the masses ($1/f^2$ power spectrum). At a high pressure [Fig. 4(c), $Pl_0=e^5$] these oscillations are dominated by the eigenfrequencies of the loop. The eigenfrequencies of small vibrations of a stretched loop of N mass points of mass m are given by $\sqrt{4\tau/(ml_0)}\sin(n\pi/[2(N+1)])$, where n runs from 1 to N, and τ is as before the tension of the connecting springs of equilibrium length l_0. We cannot expect to find exactly these frequencies in the simulation because the vibrations are strong enough for higher-order terms to become important. The dominant peak in Fig. 4(c) coincides, however, approximately (within 10%) with the eigenfrequency corresponding to $n=2$. Just below the threshold pressure, the spectra after the first impact are rather complicated mixtures of eigenfrequencies and zero-frequency modes. We will demonstrate below, however, that a transition in the average loop radius nevertheless takes place then. Near the threshold, the difference between the two free-energy minima is small, and transient behavior can appear. A collapsed loop can display local eigenfrequency oscillations, and an uncollapsed loop can have deformations with very long wavelengths. Well below the threshold, transition to the flexible state is very sharp.

C. Height of the first bounce

The elasticity of the loop can be measured by recording how high the first bounce is in comparison to the original height. For a perfectly elastic loop, this ratio (h_1/h_0) would be equal to unity. At an inelastic impact, some of the energy is transformed into work against the pressure, and into internal oscillations within the loop. This part of energy cannot be regained as potential energy in the subsequent bounces.

It is only possible for the loop to collapse completely if the energy required for a total collapse, $E_p \approx NPl_0(r_0+0.5\delta r)$, is smaller than the initial potential energy $Nmgh_0$. Here δr is the change in the loop radius as a result of the inflation, and h_0 is the height from which the loop is dropped. We would thus expect that the parameter governing the elastic behavior of the loop under impact is

$$\kappa \equiv \frac{NPl_0(r_0+0.5\delta r)}{Nmgh_0} \approx \frac{Pl_0 r_0}{mgh_0}, \tag{6}$$

where the last approximation holds for small pressures at and below the threshold.

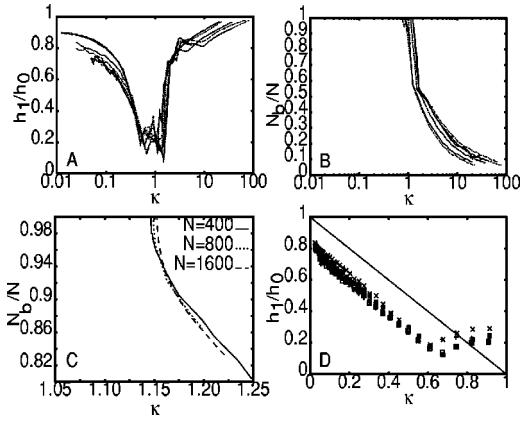

FIG. 5. (a) h_1/h_0 as a function of κ for $h_0=20,40,80$; $m=0.05,0.10,2.0$; $g=5,10,20$, and $\epsilon l_0=1000,2000,4000$. (b) N_b/N as a function of κ for the same parameters as in (a). (c) N_b/N as a function of κ for $N=400,800,1600$. (d) h_1/h_0 as a function of κ. The line is the function $1-\kappa$.

Figure 5(a) demonstrates that the simulated results for h_1/h_0 are rather well described by a single-valued function $f(\kappa)$, which has its minimum when the argument is close to 1. This minimum represents the threshold, a resonant case for which almost all of the potential energy is used for collapsing the loop at the first impact, and very little energy is left for the first bounce: h_1/h_0 reaches values as low as 0.08. To the right of the minimum in $f(\kappa)$, the loop is rigid and bounces in the uncollapsed state like an ordinary ball [cf. Fig. 1(a)]. To the left of the minimum, the loop collapses to a ''bouncing rag,'' but only a fraction of the total energy is needed for the collapse [cf. Fig. 1(b)].

D. Collapse of the loop

The collapse of the loop can also be demonstrated by considering the fraction of the mass points that touch the substrate during the first impact (N_b/N). This result is shown in Fig. 5(b). If $N_b/N=1.0$, the loop becomes completely collapsed at the first impact. For more rigid membranes N_b/N is less than 1. To demonstrate the transitionlike behavior of N_b/N, we plot this quantity for different N in Fig. 5(c). The transition between the collapsed and uncollapsed states becomes more distinct for larger N.

Based on the behavior of the energy components, the functional form of f to the left of the minimum, at $\kappa \approx 1$, can be estimated. In the region where the collapse takes place, one might guess that the energy that is transformed into in-

ternal oscillations of the membrane during the first impact is independent of P. This means that E_e+E_k at the maximum height after the first impact should be a constant c_{ke}. Since the loop completely collapses in this region, $E_p \approx NPl_0r_0$, it follows that

$$\frac{h_1}{h_0} \approx 1.0 - \frac{NPl_0r_0}{Nmgh_0} - \frac{c_{ke}}{Nmgh_0}. \tag{7}$$

c_{ke} can be obtained by recording h_1/h_0 at $P=0$. Equation (7) with $c_{ke}=0$ is plotted as a guide to the eye with simulation results in Fig. 5(d). Since c_{ke} is in fact positive, this plot lies above the simulation results. One can however see that, for at least $\kappa<0.6$, the linear approximation holds very well. The region $\kappa>0.6$ is affected by the resonant behavior associated with the threshold. Obviously collapse takes place whenever it is energetically possible, and the needed energy is removed from the c.m. kinetic energy of the loop, together with additional energy used for increased internal oscillations of the loop. This additional energy increases with increasing c.m. kinetic energy.

E. Loop radius

The bouncing loop as considered here is not in thermal equilibrium as it is not connected to a heat bath. It is thus evident that no temperature can be assigned to a rigid bouncing loop whose internal oscillations are dominated, at least for a very long time, by eigenfrequency oscillations. When the loop collapses, however, the velocity distribution of its internal oscillations turns out to assume very rapidly a Gaussian form, in fact it happens immediately after the first bounce. If we interpret this distribution as a Maxwell-Boltzmann distribution, we can assign a temperature to the collapsed loop. In leading order, this temperature corresponds, in the resonant case described above, to all of the initial c.m. potential energy transforming into internal oscillations.

We can thus think of this first bounce to rapidly heat up the loop, and thereby giving rise to an entropic contribution to its free energy as described by Eq. (2). Energy is not dissipated away from the loop so that, once created, the temperature is well defined even though it changes at the first few subsequent bounces. The situation is thus quite similar to having the loop in a heat bath. Far below the resonant case, not even subsequent bounces alter the temperature to any considerable amount. Close to resonance, the situation is more complicated, and thermalization is much slower.

In Fig. 6, we therefore compare Eqs. (3) and (4) with simulation results for $N=100,200,400$. As the temperature in Eq. (4), we use the temperature obtained from the Maxwell-Boltzmann distribution of the internal-oscillation velocities.

Transition between the two states appears to become sharper for increasing N, with excellent agreement between theory and simulations for the uncollapsed state. This is of course expected, as now the state of the loop is only determined by mechanical equilibrium. Agreement is reasonable for the collapsed state despite the several approximations involved in using Eq. (4). First of all, the temperature used in this expression is not strictly constant as in a heat bath. Also, estimating the entropy such that the structure of the membrane is that of a random walk is probably not very accurate for small systems. It is possible that for higher values of N this assumption would hold better. Qualitatively the result Eq. (4) seems to well describe the simulation results.

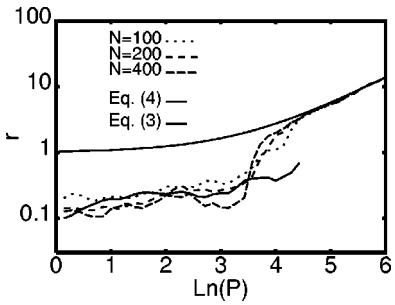

FIG. 6. The average membrane radius as measured over a few bounces as a function of inflation pressure. The analytical results Eqs. (3) and (4) are compared to simulation results for $N=100,200$, and 400.

F. Transition temperature

In order to test the theoretical free-energy prediction for the transition temperature, we consider the ratio of the temperature obtained from the Maxwell-Boltzmann distribution and the critical temperature defined by Eq. (5). This ratio is plotted in Fig. 7 as a function of κ. $T/T_c>1$ for $\kappa \lesssim 1.4$, and $T/T_c<1$ for $\kappa \gtrsim 1.4$, which means that a collapsed state should appear below $\kappa \approx 1.4$ and the rigid uncollapsed state for κ above 1.4. This is consistent with the results shown in Fig. 5(a). It thus appears that the temperature induced in the system by the impacts can indeed be interpreted as a thermodynamic temperature. It is also evident from Fig. 7 that the kinetic energy of the internal oscillations (i.e., T) depends roughly exponentially on κ above the threshold, and increases more rapidly below the threshold.

G. Long-time behavior of the rigid state

Finally, we analyze the long-time (several thousand bounces) variations in the bouncing heights at pressures clearly above the threshold. Figure 8(a) shows the trace of the center of mass of a bouncing loop over about 2500 bounces. The pressure in this case is $Pl_0=e^7$. Bouncing

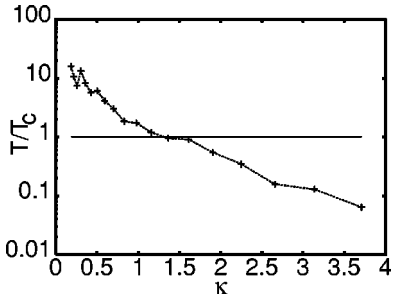

FIG. 7. T/T_c versus κ for $N=400$. The horizontal line marks the transition point.

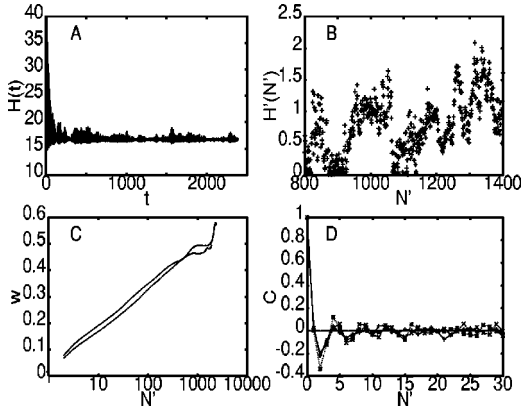

FIG. 8. (a) The height of the center of mass (H) as a function of time t. (b) Bouncing heights (H') at late times (N' is the number of bounces). (c) The average bouncing-height fluctuations w as a function of the number of bounces. (d) Correlation C of the bouncing-height differences between neighboring bounces. In (c) and (d) results are shown for two almost similar cases.

height decays considerably over the first 100–300 bounces, whereafter fluctuations dominate the behavior. The decay of the average bouncing height is roughly proportional to one over the square root of time for the first few hundred bounces.

Figure 7(b) shows the fluctuations in the bouncing height at later times. It is obvious that the heights are correlated in time and that fluctuations resemble those of Brownian motion. The structure of the bounce curve cannot however be that of the simple Brownian motion, as bouncing height is limited between the substrate and the height that corresponds to potential energy being equal to total energy. Such a constraint prevents the divergence in the average-height fluctuations, which appears in Brownian motion. Figure 7(c) shows that the average fluctuations increase roughly logarithmically with increasing number of bounces (N'), unlike the $\sqrt{N'}$ divergence for Brownian motion. This means that there must exist nontrivial correlations in the bouncing heights of adjacent bounces. Correlation functions for the differences in adjacent bouncing heights are shown in Fig. 7(d). The correlation between nearest-neighbor differences is almost zero, but for the next-nearest neighbors, correlation is clearly negative. The origin of this correlation is not known to us. A possible source for long-time correlations in the bouncing heights could be the rotational motion of the loop, which could ''store'' energy and then release it to other forms of energy. These correlation effects are, however, beyond the scope of the present work, and will be analyzed in a forthcoming publication.

IV. CONCLUSIONS

In a rigidity transition the driving parameter is the number of independent constraints. When this number exceeds the number of degrees of freedom in a system, the system becomes rigid and can resist deformation. Here the transition is different, in that we begin with an originally rigid configuration where the number of constraints is enough to fix the system in a certain shape. When a closed loop bounces, its c.m. kinetic energy is transferred into other energy components. If the average noncollective kinetic energy (i.e., internal oscillations or heat), which is thereby increased, becomes high enough, some of these constraints become marginal. If the pressure is low enough or the first impact hard enough, the loop collapses. As a collapse takes place, it becomes (because of entropic effects due to internal oscillations) favorable for the loop to be in a state where the free distance of the spring chain is as high as possible (within the boundary conditions imposed by pressure). Pressure no longer provides a set of constraints that bind the mass points to a certain distance from the center. In the rigid state we find, as expected, a set of coupled oscillators that bind the energy. The restoring forces are known for the mass points when the system is deformed. In the flexible state there are no definite restoring forces for many deformations, so the zero-energy modes, i.e., the floppy modes, dominate. There is however a collective entropy-based restoring force which keeps the average length of the spring chain or the radius of the loop constant. The dynamically driven transition is that between energetically and entropically favorable states, and it is inherently discontinuous.

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