Fluctuations and Fracture

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This Letter describes the way that metastable systems escape from traps. Brief periods during which the system apparently runs backwards in time play a crucial role. These ideas are applied to a model for one of nature's most obviously irreversible phenomena, the shattering of a body by a crack.

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In December of 1947, the *S. S. Ponagansett* suddenly cracked in half while floating quietly at its pier in Boston [1,2]. It provided dramatic evidence that macroscopic objects can irreversibly be changed by imperceptible fluctuations. The purpose of this Letter is to present a general way to calculate the likelihood of such a fluctuation, and to illustrate the formalism in a simple model of fracture.

I will show that the formal study of Hamiltonian systems in thermal baths leads one to search for trajectories in phase space which move from specified initial to specified final conditions while minimizing deviation from Newton's laws. When a metastable system escapes from a trap, initial stages of the process develop as if the system were moving backwards in time [3].

General formalism.—Consider a collection of M particles of mass m at positions x_i, moving in response to forces $F_i(x_1,\ldots,x_M)$, with velocities v_i, and which are characterized statistically by

$$g(x_1, v_1; x_2, v_2, \ldots, x_M, v_M : t). \tag{1}$$

The distribution function g gives the probability that particles i are at positions x_i with velocities v_i at time t. When placed in contact with a heat bath, this probability distribution is assumed to obey the Fokker-Planck equation [4–6]

$$\frac{\partial g}{\partial t} = \left[-\frac{\partial}{\partial x_i} v_i + \frac{\partial}{\partial v_i}\left\{-F_i + bmv_i + kTb\frac{\partial}{\partial v_i}\right\}\right] g, \tag{2}$$

where b is a phenomenological parameter describing the rate at which thermal equilibrium establishes itself, k is Boltzmann's constant, and T is the temperature.

Equation (2) is of a form whose solution may be represented by a functional integral [7]. A brief calculation shows that the probability of a state beginning at $\vec{x}^0, \vec{v}^0$ and ending at $\vec{x}^f, \vec{v}^f$ after time τ is

$$g(\vec{x}^f, \vec{v}^f : \tau) = \int \mathcal{D}x\, e^{-\int_0^\tau dt \sum_i [m\ddot{x}_i - F_i + mb\dot{x}_i]^2/4mkTb}. \tag{3}$$

In Eq. (3) the integral is over all paths having the property that

$$x_i(0) = x_i^0 \quad \text{and} \quad \dot{x}_i(0) = v_i^0, \tag{4}$$

$$x_i(\tau) = x_i^f \quad \text{and} \quad \dot{x}_i(\tau) = v_i^f. \tag{5}$$

The argument of the exponential in Eq. (3) has a nice physical interpretation. It says that the most important thermal histories are those which minimize deviation from Newton's laws.

I now assume that the functional integral in Eq. (3) is dominated by a single path which maximizes the integrand [8]. The approximation to be explored, therefore, is

$$g(\vec{x}^f, \vec{v}^f : \tau) \sim e^{-U(\tau)/kT}, \tag{6}$$

where the activation barrier $U(\tau)$ is

$$U(\tau) = \min_{\vec{x}(t)} \int_0^\tau \frac{dt}{4mb} \sum_i D_i^2, \tag{7}$$

with the deviation D_i from Newtonian mechanics

$$D_i(t) \equiv m\ddot{x}_i - [F_i - mb\dot{x}_i]. \tag{8}$$

The minimization in Eq. (7) is carried out over all paths $\vec{x}(t)$ starting and ending with the positions and velocities required by Eqs. (4) and (5).

Two types of minima of Eq. (7) can be understood analytically. The first is a path $x_i^{\text{Newt}}(t)$ which obeys Newton's laws, so that $D_i(t) = 0$. The activation barrier U associated with this sort of path is zero, but it cannot in general satisfy both boundary conditions Eqs. (4) and (5). In particular, such paths cannot solve problems in which systems escape from local energy minima, since the damping in Eq. (8) requires energy to decrease as t moves from 0 to τ. A second class of minima is obtained by taking any solution $x_i^{\text{Newt}}(t)$, and running it backwards in time. It is easy to check that $x_i^{\text{Newt}}(\tau - t)$ solves the Euler-Lagrange equations which follow from minimizing U in Eq. (7), and that the activation barrier U resulting from such a path is

$$U = 2b \int_0^\tau dt \sum_i \frac{m}{2} (\dot{x}_i^{\text{Newt}})^2. \tag{9}$$

Paths of this second type can start at the bottom of an energy well at $t = 0$, and evolve towards some higher energy at $t = \tau$. It is therefore natural to guess that the best way to escape from a trapping potential is for a system to follow a path of this second type from $t = 0$ until some intermediate time τ_1, at which point the system has reached the top of the barrier which restrains it. Now the system can switch over to a path of the first type,

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and further deterministic evolution, carrying no additional contributions to U, will take it to the desired final state. This guess captures the essential feature of solutions of Eq. (7), although numerically obtained solutions actually switch somewhat gradually from moving "backwards" in time to moving "forwards" in time, not abruptly as this argument would indicate.

Application to fracture.—Fracture provides a natural context in which to explore this general formalism, since it connects the spontaneous failure of atomic bonds to macroscopic failure of a body. The classic theory [9], going back to Griffith [10], holds that as the load on a body increases rapid fracture should reproducibly occur at a definite critical value, the Griffith point. This picture lacks clean experimental verification in brittle materials, and also leads to interesting conceptual problems [11]. By contrast, recent studies from an atomic point of view [12,13] find that there is no Griffith point. The bifurcation is really subcritical; at a given value of loading, both stationary and rapidly moving cracks might be possible. Analogy with first-order phase transitions immediately suggests that one take up the statistical problem of the jump from stationary states to rapidly moving ones. Simultaneously, one is led to consider the separate physical process of creep (observed, for example, in damaged car windshields) in which a crack gradually inches forward, although never acquiring substantial velocities.

In order to use Eq. (2) for this physical problem, one must find an appropriate collection of forces F_i. A particularly simple case is illustrated in Fig. 1 and defined by the equations

$$F_i = \begin{cases} x_{i+1} - 2x_i + x_{i-1}, & \text{coupled to neighbors,} \\ +\frac{1}{N}(\Delta\sqrt{2N+1} - x_i), & \text{driving term,} \\ -2x_i\theta(1 - x_i), & \text{bonds which snap.} \end{cases} \tag{10}$$

Placing Eq. (10) into Eq. (2), one models a thin strip of cracked material under stress, suffering bombardments on all sides from molecules which maintain it at temperature T.

Many features of Eq. (10) have been worked out previously [12–14]. The main results are the following: (1) For fixed driving term Δ, most behavior becomes independent of N in the limit where the model mimics a microscopic crack in a macroscopic strip, the limit of large N. (2) There are linearly stable, stationary crack solutions for a wide range of Δ. In the limit of large N, the range is from $\Delta = (\sqrt{3} - 1)/\sqrt{2} = 0.51\ldots$ to $\Delta = (\sqrt{3} + 1)/\sqrt{2} = 1.93\ldots$. (3) A branch of stable steadily moving solutions begins at around $\Delta \approx 1.2$, and $v = v_{\min} \approx 0.3$, with v increasing as Δ increases. There are no steady-state solutions at all for $0 < v < v_{\min}$.

The goal is to understand how a stable stationary crack can be knocked out of complacency by thermal fluctuations

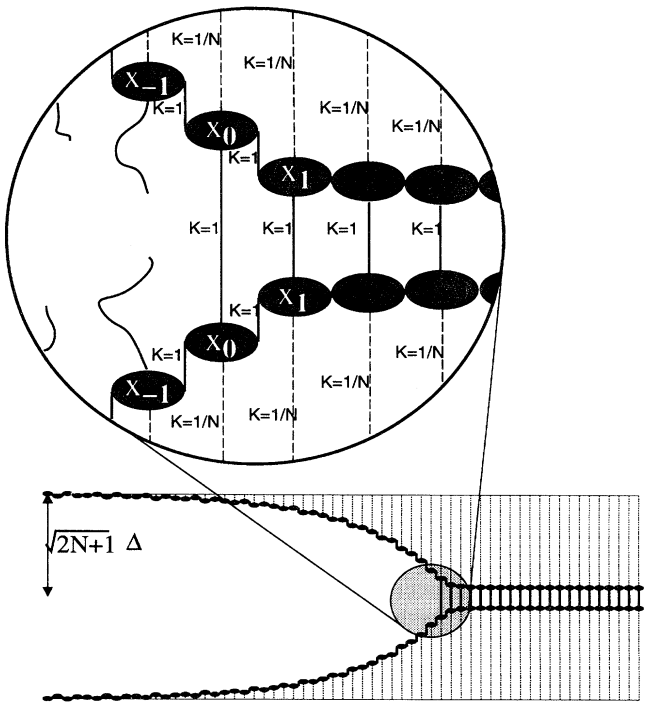

FIG. 1. This one-dimensional model mimics the motion of a crack in a strip, incorporating effects of discreteness. One can view it as a model for the atoms lying just along the surface of a crack. Above these atoms lie N additional lines of atoms, which are, however, massless and do not enter as degrees of freedom. Mass points are only allowed to move vertically, and are tied to their vertical neighbors with springs which break when they exceed unit extension. The lower portion of the figure shows an actual steadily moving solution of the model with velocity $v = 0.5$. Only cases where the mass points move perfectly symmetrically about the crack line will be considered; Eq. (10) does not treat the upper and lower masses as separate degrees of freedom.

and made to creep, or to run. Creep is slightly easier to understand. A single creep event constitutes a configuration which is stationary and stable at $t = 0$, and again stationary and stable a large time later at $t = \tau$, but moved precisely one lattice spacing to the right. The optimal path leading to this event can be generated by grabbing the two masses labeled by index 0 in Fig. 1 and pulling them slowly apart until the bond connecting them is on the verge of snapping. A slight impulse delivered to these central masses causes the bond to sever, and, if the masses are now released, there is a range of Δ for which the subsequent time evolution causes the crack to relax into a stationary configuration one lattice point ahead. On the other hand, if the masses are released before the bond severs, the whole crack relaxes back to the original configuration. The time reverse of this latter relaxation, glued onto the evolution which severs a bond and moves the crack forward constitutes a creep event. A solution of this type, generated by numerical minimization of Eq. (7), appears in Fig. 2 [15].

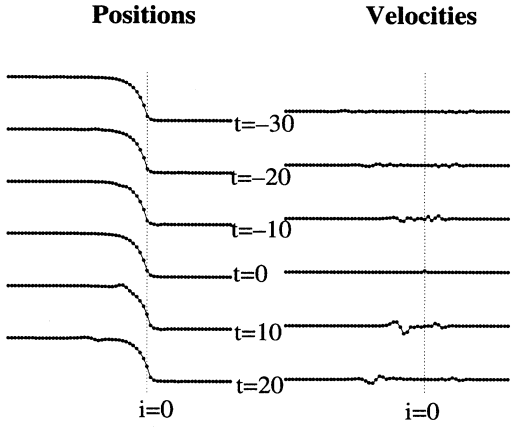

FIG. 2. A creep event obtained from numerical minimization of Eq. (7), for model Eq. (10) with $N = 9$, $\Delta = 1.2$, and $b = 0.1$. Time $t = 0$ is chosen as the instant that the bond at the crack tip snaps. At large negative times the crack is stationary. Traveling waves spontaneously appear far from the tip, and travel towards it, growing as they move. They strike the tip in perfect synchrony, snapping the bond at the tip so that its velocity has dropped to zero as it snaps. The crack sheds waves as it relaxes to its new stationary configuration, one site to the right.

To calculate creep rates analytically, start with a stationary crack in equilibrium [13], and imagine applying forces to the masses nearest the crack tip, pulling them apart adiabatically until the bond between them has reached unit length and is ready to break. Denote the energy put into the system during this process by E_{pull} [16]. Assuming that b is small, using the virial theorem, and the fact that relaxing solutions decay as $e^{-bt/2}$, one finds from Eq. (9) the estimate that the activation energy for creep is

$$U = E_{\text{pull}}. \tag{11}$$

Detailed numerical solutions produce activation barriers consistent with this estimate, as shown in Fig. 3. Considering the probability of many consecutive creep events randomly spaced in time, leads to the prediction that the crack creep velocity $\dot{l}$ is

$$\dot{l} \sim e^{-U/kT}. \tag{12}$$

This expression is in perfect accord with phenomenological expressions for creep rates [17], and with previous theoretical estimates [18].

For a range of driving strain Δ, a stationary crack may encounter an especially large thermal fluctuation which drives it into rapid motion. Such a jump event is depicted in Fig. 4. The difference in this case between creeping and jumping is that at the instant the first bond snaps, the central mass possesses a rather large momentum, and as a consequence the crack is able to run forever. If Δ is less than 1.198... such jump events are impossible, but once Δ becomes large enough, creep is no longer favorable, and all cracks run as soon as a single bond snaps.

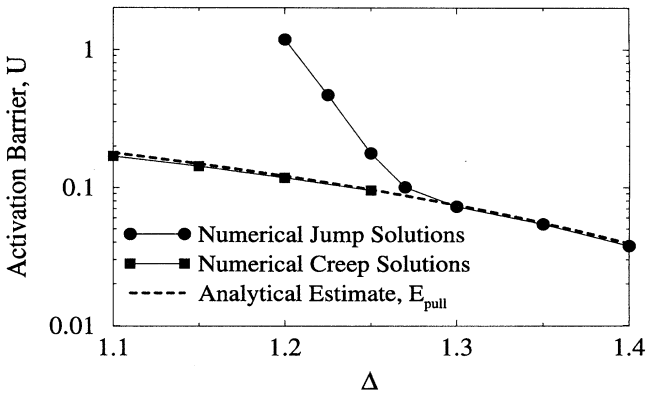

FIG. 3. Results of a numerical search for minimum activation energies, U, as a function of Δ. The circles show the activation barrier of creep events, the squares show the activation barrier of jump events, and the thick dashed line shows a plot of the estimate Eq. (11). All the calculations are carried out for $N = 9$ and $b = 0.1$. At low strains Δ, only creep events are possible. For $\Delta = 1.198$ jump events first become possible, although their activation barrier is initially very high. By the time $\Delta \approx 1.3$, jump events occur immediately if even a single bond snaps, and creep is no longer possible.

These results are summarized in Fig. 3, which shows the activation energies of creep events and jump events as a function of Δ for a particular value of N and b. The region where creeping and jumping can coexist is quite small, but I suspect that improvements of model Eq. (10) will make this region larger.

Although Eq. (2) invokes only thermal fluctuations to trigger jump and creep events, in practical situations nonthermal noise and chemical attack are crucially important [19]. The modeling must be improved to compare with experiment. However, I would prefer to close with observa-

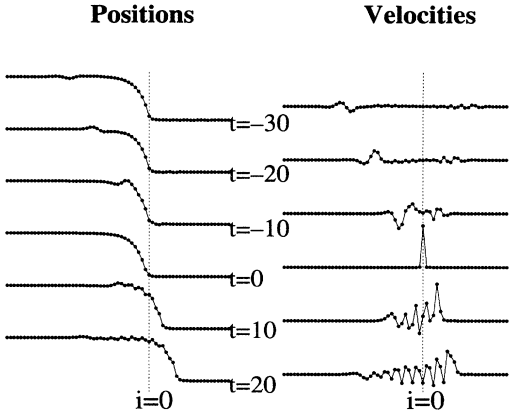

FIG. 4. A jump event obtained from numerical minimization of Eq. (7), for model Eq. (10) with $N = 9$, $\Delta = 1.2$, and $b = 0.1$—precisely the same values as in Fig. 2. However, one now imposes final boundary conditions $\vec{x}^f$ and $\vec{v}^f$ corresponding to a running crack, and the fluctuations D_i arriving at the crack tip must be larger than in the previous case to achieve them.

tions on how the conceptual picture illustrates the direction of time [20]. Consider the dissipationless limit $b \to 0$ in which all behavior becomes completely reversible. It appears that if one finds a rapidly running crack, takes every mass and sends $v_i \to -v_i$, the crack will then run backwards and close up [21]. Indeed, according to Liouville's theorem, the phase space of initial conditions leading to crack healing must be of the same size as the phase space leading to crack separation, so should not bodies which spontaneously heal themselves be as common as those which shatter? A glance at Fig. 4 may help provide the answer. The forward motion of a crack involves emission of waves which travel to the far reaches of the system. For the crack to be able to travel backwards and heal itself, one has to arrange for these waves to arrive from far away in exponentially perfect synchrony. It does little good to know that the phase space of solutions which heals the crack has a certain volume, if that volume is thin as strands of a spider's web, and dispersed in the far reaches of the Universe. Nevertheless, solutions of this type are crucial, since decay cannot occur without such backwards-moving eddies in the flow of time.

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