PHYSICAL REVIEW E VOLUME 54, NUMBER 4 OCTOBER 1996

Statistical mechanics of cracks

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(Received 14 May 1996)

This paper describes a formalism designed to answer questions about Hamiltonian systems in contact with a heat bath. The formalism is applied to a simple model of fracture to find, first, the rate at which a crack creeps through a brittle body as a result of thermal fluctuations and, second, the rate at which the crack jumps from creeping to rapid motion. The dominant exponential behavior of these processes is calculated exactly, but the prefactors are only estimated. Some of the solutions cannot be viewed in the traditional manner as corresponding to passage over a saddle point. Viewed as an isolated Hamiltonian system, the crack shows that irreversible behavior can arise because, although the probability of traveling from past to present equals the probability of traveling backwards from present to past, the probabilty of traveling still further into the future is exponentially greater. [S1063-651X(96)06410-0]

PACS number(s): 05.70.Ln, 82.20.Db, 62.20.Mk, 46.30.Nz

I. INTRODUCTION

A. Motivation

One of the intriguing paradoxes in physics is the conflict between the symmetry of mechanics with respect to reversal of the sign of time and the obvious absence of this symmetry in the everyday world. For this reason, it is interesting to study irreversible phenomena at the atomic level.

Fracture provides a natural context in which to explore this general problem, since it connects the spontaneous failure of atomic bonds to macroscopic failure of a body. This paper will focus upon two statistical problems in fracture. The first is that of creep, which occurs, for example, during the long slow progress of a crack across a car windshield. Creep fracture is widely studied [1], has been examined experimentally with great care, and is described by good phenomenological expressions which accord well with the data. The second problem is that of rapid fracture initiation, in which an object suddenly shatters without apparent cause. Although related to something called static fatigue in the engineering community, this phenomenon is not widely known. The calculations I will describe are much more detailed than any previous descriptions, first showing how the familiar phenomenological rules arise from microscopic laws and then generalizing and improving upon them.

To make more specific the setting of these problems, imagine placing a single crystal strip of silicon in a controlled environment at temperature T [2]. The strip contains a long crack down the center, as shown in Fig. 1, and is gripped by clamps that rigidly displace the upper and lower boundaries. For a range of displacements, the crack creeps forward at a rate that depends exponentially on the temperature and might be of order μm/sec. If the displacement is high enough, the crack may begin suddenly to move at over 1000 m/sec and its velocity is largely independent of temperature. This onset of rapid motion arises in a statistical fashion as a result of thermal fluctuations and is not guaranteed to occur immediately at a critical tension.

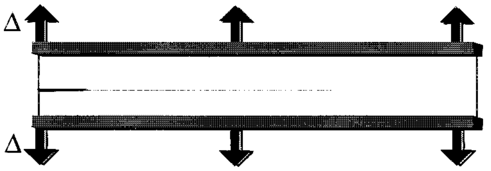

FIG. 1. A crack lies in the center of a strip whose upper and lower boundaries have rigidly been displaced from their equilibrium locations by an amount Δ.

In order to address these problems, it is necessary to devise a formalism capable of starting with an arbitrary classical mechanical system, coupling it with a heat bath, finding the probability of starting with some initial configuration in phase space, and ending with some other specified configuration in phase space. This task is accomplished using functional integrals and results eventually in expressions for creep and rapid fracture initiation rates for a simple model system. For several different reasons, however, realistic comparison with experiment will demand additional layers of complexity, which I have not yet begun to incorporate.

B. Organization of the paper

Because this paper is fairly long and contains results of many different types, I summarize the main points.

II A. This section recalls a formalism, due to Kramers, that casts all of classical mechanics into a statistical form.

II B and Appendix A. These sections derive a complete formal solution of Kramers's equation using a functional integral.

II C. This section extracts from the functional integral a variational principle useful for accurate calculations at low temperatures, and finds three special solutions. The first corresponds to a system evolving deterministically forward in time. The second corresponds to a system evolving deterministically backward in time.

II D. This section shows that the third special solution results from gluing together the first two types of solutions sequentially. An activated process is described by transition-state theory (passes over a saddle point) if and only if it is a solution of this third type.

III A. The nature of static and dynamic cracks is fundamentally affected by the atomic structure of matter.

III B. This section reviews a simple one-dimensional model of fracture.

III C. This section displays an explicit solution of the variational problem for creep rates. The answer is identical to transition-state theory.

III D. This section finds a numerical solution of the variational problem for cases which cannot be described by transition-state theory (no saddle point) and obtains the low-temperature phase diagram for the model system.

III E. this section extracts the creep rate from the probability of breaking one bond.

IV A. This section discusses the significance of systems traveling backward in time.

IV B. This section contains reflections upon time-reversal invariance. Asymmetry in time results from the basic asymmetry involved in preparing an irreversible event.

V A and Appendix B. These sections generalize the path decomposition expansion of Auerbach and Kivelson.

V B. This section applies the decomposition to estimate Gaussian prefactors.

VI. The paper concludes with reflections upon the further work needed before comparison with experiment becomes possible.

II. FUNCTIONAL INTEGRAL FOR HAMILTONIAN SYSTEMS

A. Fokker-Planck equation

Suppose one has a Hamiltonian system consisting of M particles of mass m, obeying

$$\dot{p}_i = -\frac{\partial \mathcal{H}}{\partial x_i} = F_i(\vec{x}) \tag{1a}$$

$$\dot{x}_i = \frac{\partial \mathcal{H}}{\partial p_i} = \frac{p_i}{m}. \tag{1b}$$

Consider the probability distribution

$$g^{\tau}_{0\to n} = g(\vec{x}\vec{p};\tau), \tag{2}$$

which gives the probability that the system will begin in an initial configuration where the positions and momenta of the particles are $\ldots, x^0_{-1}, p^0_{-1}, x^0_0, p^0_0, x^0_1, p^0_1 \ldots$ and end time τ later with positions and momenta of the particles at new values $\vec{x}\vec{p} = \vec{x}^n\vec{p}^n$.

Particle locations and momenta obey the convention that subscripts label the particle number, while superscripts are used to indicate values of positions and momenta at different times. $\vec{x}\vec{p}$ and $\vec{x}^n\vec{p}^n$ will be used interchangeably to indicate the positions and momenta at time τ.

When placed in contact with a heat bath, g obeys the equation

$$\frac{\partial g}{\partial \tau} = \sum_i \left[-\frac{\partial}{\partial x_i}\frac{p_i}{m} + \frac{\partial}{\partial p_i}\left\{ -F_i + bp_i + mkTb\frac{\partial}{\partial p_i} \right\} \right] g. \tag{3}$$

If the damping constant b is set to zero, Eq. (3) simply expresses Hamilton's equations (1) for the distribution function g. If the damping constant b is nonzero, the presence of a heat bath causes the momentum of each particle to diffuse. The terms proportional to b have been chosen so that

$$g \sim e^{-\mathcal{H}/kT} \tag{4}$$

is a static solution of Eq. (3), with k Boltzmann's constant and T the temperature; in accord with the fluctuation-dissipation theorem, the first term proportional to b describes linear damping of particles, while the second term proportional to b describes the effect of a fluctuating thermal bath.

The Fokker-Planck equation (3), due to Kramers [3], is discussed in detail by van Kampen [4] and Hänggi, Talkner, and Borkovec [5] and is conventionally felt to provide a trustworthy representation of any classical mechanical system under the influence of the heat bath. Nevertheless, it has two worrisome features. First, one might wonder about the legitimacy of phenomenological damping at the atomic level. This worry is relieved by the facts that the limit $b \to 0$ is perfectly well defined in all final expressions and that one is free to allow b to vary in space; in particular, one can take b to be nonzero only on the boundaries of the system. Second, Eq. (3) neglects quantum mechanics. This objection is legitimate, since calculations by Gilman and Tong [6] show that quantum-mechanical tunneling is considerable at low temperatures. Thus the calculations in this paper apply only to temperatures high enough that quantum-mechanical coherence is unimportant.

B. Functional integral formulation

The technique of functional integration allows one to find an exact formal solution of Eq. (3). Casting the Fokker-Planck equation into the form of a functional integral requires a brief calculation that closely mirrors familiar procedures [7,8] and is recorded in Appendix A. The result of this appendix is an expression for the time evolution of g in the form

$$g^{\tau}_{0\to n} = \int Dx^{n-1} g^{\tau-dt}_{0\to n-1} G_{n-1\to n}, \tag{5}$$

where

$$Dx^l = \prod_i \left\{ dx^l_i \sqrt{\frac{m}{4\pi kTb\,dt^3}} \right\}, \tag{6}$$

$$G_{n-1\to n} = \exp\left\{ -dt \frac{\sum_i \left[\frac{p^n_i - p^{n-1}_i}{dt} - (F_i - bp^{n-1}_i) \right]^2}{4mbkT} \right\}, \tag{7}$$

and

$$p^l_i \equiv m\frac{x^{l+1}_i - x^l_i}{dt} \quad \text{for} \quad 1 \leqslant l \leqslant n-1. \tag{8}$$

This notation leads to compact expressions, but risks being misleading, since $p^n_i = p_i$ and p^0_i are independent variables specifying momenta of particles at initial and final times, but for all other superscripts l, p_i^l is defined completely in terms of x_i^l and x_i^{l+1} by Eq. (8).

Taking $\tau=(n-1)dt$ and using Eq. (5) repeatedly, one then finds that

$$g_{0\to n}^{\tau}=\int\left(\prod_{l=1}^{n-1}Dx^l G_{l\to l+1}\right)\delta(\vec{x}^1-\vec{x}^0)\,\delta(\vec{p}^1-\vec{p}^0) \qquad (9)$$

or

$$g(\vec{x}\vec{p};\tau)=\int\mathcal{D}x\ \exp\left(-\int_0^{\tau}dt\sum_i\ [\ddot{x}_i-F_i+b\dot{x}_i]^2/4mkTb\right). \qquad (10)$$

The functional integral $\int\mathcal{D}x$ is over all paths $\vec{x}(t)$ that begin with the desired initial values of

$$\vec{x}(0)=\vec{x}^0,\quad m\dot{\vec{x}}(0)=\vec{p}^0 \qquad (11a)$$

and end with the desired final values of

$$\vec{x}(\tau)=\vec{x},\quad m\dot{\vec{x}}(\tau)=\vec{p}. \qquad (11b)$$

Equation (10) is an exact formal solution of Eq. (3), but its main practical value is as a starting point for approximate expressions at low temperatures.

C. Variational principle at low temperatures

At low temperatures, the functional integral is dominated by a single classical path $\vec{x}(t)$ that maximizes the integrand. This path is the one that minimizes the functional

$$S[\vec{x}(t)]=\int_0^{\tau}\frac{dt}{4mb}\sum_i\ [m\ddot{x}_i-(F_i-mb\dot{x}_i)]^2, \qquad (12)$$

so the probability of going from initial state 0 to final state n is

$$e^{-U/kT}, \qquad (13)$$

where

$$U=\min_{\vec{x}(t)}S[\vec{x}(t)], \qquad (14)$$

subject to the boundary conditions (11). Thus one arrives at the physically satisfying result that the most likely way to move from one configuration to another is to minimize the deviation from Newton's laws of motion, in the presence of a small amount of damping.

Define $D_i(t)$ to be the deviation from Newton's laws

$$D_i(t)\equiv m\ddot{x}_i-F_i+mb\dot{x}_i\,. \qquad (15)$$

Then the Euler-Lagrange equations that locate extrema of Eq. (12) are

$$0=m\ddot{D}_i-\sum_j\frac{\partial F_i}{\partial x_j}D_j-mb\dot{D}_i\,. \qquad (16)$$

One can guess two exact solutions of Eq. (16). Clearly, no path could give a lower value of S than any $\vec{x}(t)$ that satisfies

$$m\ddot{\vec{x}}=\vec{F}(\vec{x})-mb\dot{\vec{x}}, \qquad (17a)$$

with

$$\vec{x}(0)=\vec{x}^0,\quad m\dot{\vec{x}}(0)=\vec{p}^0. \qquad (17b)$$

Such a path leads to

$$D_i=0\ \text{ and hence }\ S[\vec{x}]=0. \qquad (18)$$

Unfortunately, paths of this type do not provide all the necessary minima of S because they can be chosen to satisfy one but not both sets of boundary conditions Eqs. (11).

One can also find a second class of exact solutions of Eq. (16). These are paths that satisfy

$$m\ddot{\tilde{\vec{x}}}=\vec{F}(\tilde{\vec{x}})+mb\dot{\tilde{\vec{x}}}, \qquad (19a)$$

with

$$\tilde{\vec{x}}(\tau)=\vec{x},\quad \dot{\tilde{\vec{x}}}(\tau)=\vec{p}/m, \qquad (19b)$$

which is identical to Eq. (17a), except that the sign of time has been reversed. To see that any function solving Eq. (19a) also solves the Euler-Lagrange equation (16), simply differentiate (19a) with respect to time. Then

$$0=\frac{d}{dt}[m\ddot{\tilde{x}}_i-F_i-mb\dot{\tilde{x}}_i] \qquad (20)$$

$$\Rightarrow 0=m\ddot{\tilde{v}}_i-\sum_j\frac{\partial F_i}{\partial\tilde{x}_j}\tilde{v}_j-mb\dot{\tilde{v}}_i\,, \qquad (21)$$

where

$$\tilde{v}_i=\dot{\tilde{x}}_i\,. \qquad (22)$$

However, one sees immediately that Eq. (19a) implies

$$\tilde{D}_i=m\ddot{\tilde{x}}_i-F_i+mb\dot{\tilde{x}}_i=2mb\tilde{v}_i\,. \qquad (23)$$

Therefore, Eqs. (16) and (21) are the same and a solution of (19a) also solves the Euler-Lagrange equations. The action S corresponding to this solution is

$$S[\tilde{x}(t)]=b\int_0^{\tau}dt\sum_i\ m\dot{\tilde{x}}_i^{\,2} \qquad (24)$$

$$=\int_0^{\tau}dt\sum_i\ \dot{\tilde{x}}_i\left[F_i+bm\dot{\tilde{x}}_i+\frac{\partial V}{\partial\tilde{x}_i}\right] \qquad (25)$$

$$=\int_0^{\tau}dt\sum_i\ \left[m\dot{\tilde{x}}_i\ddot{\tilde{x}}_i+\dot{\tilde{x}}_i\frac{\partial V}{\partial\tilde{x}_i}\right] \qquad (26)$$

$$=\int_0^{\tau}dt\frac{d}{dt}\left[\sum_i\ \frac{1}{2}m(\dot{\tilde{x}}_i)^2+V(\tilde{\vec{x}})\right] \qquad (27)$$

$$=E(\tau)-E(0)\equiv U_c\,, \qquad (28)$$

where $V(\tilde{\vec{x}})$ is the potential energy and $E(t)$ is the total energy of the system at time t.

D. Gluing solutions together

One can create additional solutions by ‘‘gluing together’’ solutions of these two types. From $t=0$ until $t=\tau_1$ a system can evolve ‘‘backward’’ in time, according to Eq. (19a), and at $t=\tau_1$, with all positions and momenta continuous, it can begin to evolve ‘‘forward’’ in time, according to Eq. (17a). While solutions of the four-point boundary-value problem described by Eq. (11) cannot generally be obtained in this way, many physically interesting solutions are of this character. All the contributions to their action come from the initial segments where the system goes backward in time, so the probability of such a path is determined by the energy barrier U_c defined in Eq. (28). To find a minimum action path of this type, it is sufficient to find some saddle-point configuration $[\vec{x}^s,\vec{p}^s]$, such that

$$\begin{aligned}&[\vec{x}^0,\vec{p}^0] \text{ evolves via } \tilde{x}(t) \text{ to } [\vec{x}^s,\vec{p}^s],\\ &\text{which evolves via } x(t-\tau_1) \text{ to } [\vec{x},\vec{p}].\end{aligned} \tag{29}$$

So the minimum action path is proposed to be

$$\theta(\tau_1-t)\tilde{\vec{x}}(t)+\theta(t-\tau_1)\vec{x}(t-\tau_1), \tag{30}$$

assuming that $\tilde{x}$ and x can be found to obey the boundary conditions indicated in (29).

A function of the form (30) provides an exact solution of Eq. (16) under the condition that

$$\ddot{\tilde{\vec{x}}}(\tau_1)=\ddot{\vec{x}}(0)=\vec{0}, \quad \tilde{\vec{p}}(\tau_1)=\vec{p}(0)=\vec{0}, \tag{31}$$

which means that the saddle point at $\tilde{x}(\tau_1)$ is an equilibrium point. Demonstrating that Eq. (30) is then an exact solution is quite simple; use Eqs. (18) and (23) for D and $\tilde{D}$ and substitute (30) into (16). However, there is a slight subtlety. A path that satisfied Eq. (31) exactly at τ_1 would remain trapped there for all time; one must actually consider a sequence of paths, which converges to one obeying Eq. (31), passing over the saddle point with increasingly negligible velocities.

In studying physical processes that require fluctuations to take the system over an energy barrier, transition-state theory [3,5] asserts that the probability of an activated process crossing an energy barrier of height U_c must be proportional to

$$e^{-U_c/kT}. \tag{32}$$

We have recovered precisely this result for paths of the form (30). The long and complicated passage of the physical system through phase space is unimportant and only the rise in energy needed to reach the saddle point matters in the end. However, suppose that one chooses initial and final configurations in phase space for which it is impossible to find a path of the form (30) also obeying Eq. (31) at some intermediate time. The simplifications leading to transition-state theory are lost and I have found no compact alternative to Eq. (12). The familiar mental picture of a system escaping over a barrier no longer applies quantitatively. The slow creep of cracks provides an example of a process that obeys Eq. (31), while the jump of cracks from stationary to moving configurations provides an example that sometimes cannot.

III. APPLICATION TO FRACTURE

A. Background

The classic theory of fracture [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. However, work by Thomson and collaborators [11–13] showed that this picture is not really correct. The tip of a crack in a crystal can become trapped at a lattice site for a range of externally imposed stresses. The phenomenon is referred to as ‘‘lattice trapping’’ and is very similar to pinning phenomena in other cases, such as charge-density waves.

The study of lattice trapping concerns only stationary cracks. The analytical study of moving cracks in lattices was initiated by Slepyan and co-workers [14,15], who found that crack motion inevitably involves the emission of high-frequency phonons. Although the complete story of how cracks move in crystals is a complicated one and has not yet fully been deciphered, some additional points now seem clear [16,17].

The zero-temperature phase diagram for cracks in brittle crystals is indicated on the top in Fig. 2. The diagram describes steady-state cracks in a strip, controlled by a dimensionless parameter Δ, which measures how far apart one has pulled the top and bottom of the strip, and which is normalized to equal 1 at the Griffith point. This parameter will be defined for a particular model in Eq. (33); in fracture mechanics terminology [12] $\Delta=K_I/K_{Ic}$. The subject of this paper is the lower portion of Fig. 2. At nonzero temperature, lattice-trapped cracks are not stationary, but creep forward at a rate that grows exponentially with temperature. In addition, they can jump at some rate up to the branch of rapidly moving cracks. The goal is to calculate these two rates. This problem is somewhat similar to that of Brownian motion in biased periodic potentials (see Ref. [5], p. 303), but acquires some new features due to the inclusion of a very large number of degrees of freedom.

B. Simple one-dimensional model

In order to use Eq. (3) for this physical problem, one must find an appropriate collection of forces F_i. A particularly simple case is illustrated in Fig. 3 and defined by the equations

$$F_i=\begin{cases} x_{i+1}-2x_i+x_{i-1} & \text{(coupled to neighbors)},\\ +\dfrac{1}{N}(\Delta\sqrt{2N+1}-x_i) & \text{(driving term)},\\ -2x_i\theta(1-x_i) & \text{(bonds that snap)}.\end{cases} \tag{33}$$

Placing Eq. (33) into Eq. (3), one models a thin strip of

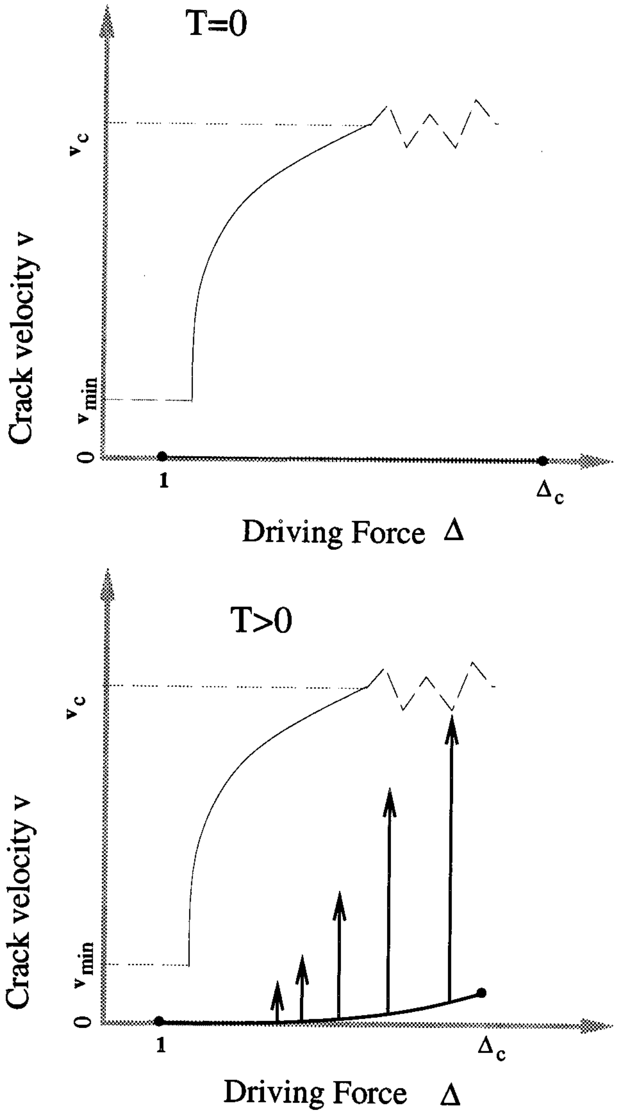

FIG. 2. Schematic phase diagram for cracks in brittle lattices, as deduced from analytical solutions of lattice models. Δ is a dimensionless measure of the external driving force on the system. On the top is the situation at zero temperature. Cracks at zero velocity are stable for a range of Δ; this is the phenomenon of lattice trapping. However, for some of the same values of Δ, rapidly moving cracks are also possible. The minimum velocity at which they can move is $v_{\rm min}$, and they become unstable at v_c to a nonlinear instability that I will not consider at all in this paper. On the bottom is the situation at nonzero temperature. The main change occurs in the lattice-trapped branch of solutions. These move at nonzero rate for any $\Delta > 1$. In addition, they make transitions at some rate to the upper branch of solutions. Calculating these two rates is the subject of this paper.

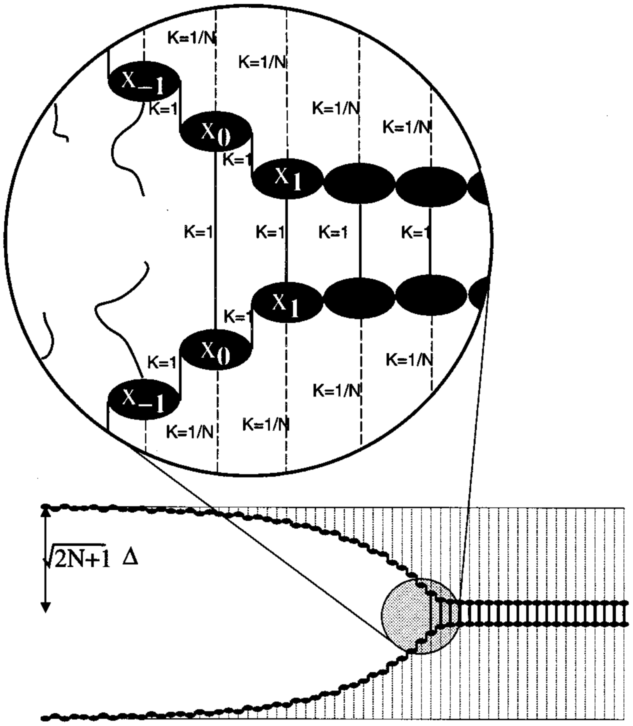

FIG. 3. This one-dimensional model mimics the motion of a crack in a strip, incorporating effects of discreteness. One can view it as a model for the atoms lying just along the surface of a crack. The mass points are only allowed to move vertically and are tied to their neighbors with springs that break when they exceed a certain 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 symmetrically about the crack line will be considered.

cracked material under stress, suffering bombardments on all sides from molecules that maintain it at temperature T.

Many features of Eq. (33) have been worked out previously [16–18]. The main results correspond to the qualitative picture in Fig. 2, except that the nonlinear instability at v_c is not present in this one-dimensional case. Some of the mathematical conclusions are the following.

(i) 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.

(ii) 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 $\Delta = (\sqrt{3}+1)/\sqrt{2} = 1.93\ldots$.

(iii) A branch of stable steadily moving solutions begins at around $\Delta \approx 1.2$ and $v = v_{\rm min} \approx 0.3$, with v increasing as Δ increases. There are no steady-state solutions at all for $0 < v < v_{\rm min}$.

C. Creep processes

As a first application of the formalism of Sec. II B, consider the process of thermally activated creep of a crack. A crack originally trapped at some lattice site snaps an atomic bond, jumps ahead by one lattice spacing, and ends stationary one site further to the right. To calculate the probability of such an event, use the formalism of Sec. II B with the initial condition of a stationary crack and the final condition, a long time later, of the same stationary crack displaced by one site to the right.

It is easy to guess the saddle point the crack must cross in moving from initial to final configurations. Imagine grabbing the two masses labeled x_0 in Fig. 3 and slowly and symmetrically pulling them apart until the distance between them is just shy of 1. If the external force is now released, the crack will relapse back into its original configuration. However, the slightest additional pull will snap the vertical bond and even upon releasing the external force the crack will certainly move forward. Whether the crack will move forward by only one bond at this point or take off running forever can be settled only by detailed calculations. There is a range of Δ for which the crack moves ahead by only one bond and then stops and we will focus on this possibility for the moment.

The definition of the model given in Eq. (33) does not really describe the saddle point over which the system passes during creep. The saddle point occurs when $x_0 = 1$ and the Heaviside θ function is ambiguous there. The proper way to think about this technical point is to replace the θ function by one that passes continuously from 1 to 0 as x_0 rises from below to above 1, over a very small range of x_0. I have made this replacement in all numerical work. Somewhere in the midst of this tiny range is an unstable equilibrium, which is the true saddle point. Physical results seem to be independent of the way the width of this region is taken to go to zero.

Therefore the configuration $[\vec{x}^s, \dot{\vec{x}}^s]$ described in Sec. III B corresponds here to the case in which an external force applied to x_0 brings it to height 1, all masses points except the one at $i = 0$ are stationary, and $\dot{x}_0^s$ is extremely small and positive. An explicit description of this state is

$$x_i^s = \begin{cases} \dfrac{\Delta}{\sqrt{2N+1}}(1-z^i) + z^i & \text{for } i \geqslant 0, \\ \Delta\sqrt{2N+1}(1-y^i) + y^i & \text{for } i < 0, \end{cases} \tag{34a}$$

where y and z are constants being raised to the ith power, which solve the quadratic equations

$$y - 2 + 1/y - 1/N = 0 \tag{34b}$$

and

$$z - 2 + 1/z - 2 - 1/N = 0. \tag{34c}$$

The total energy required to raise a stable static crack to this state is given by the integral of the force on mass 0 over the distance it has to move and is

$$U_c = \frac{(A-B)^2}{2B}, \tag{35}$$

with

$$A = \Delta\left(\sqrt{2N+1} - \frac{1}{y\sqrt{2N+1}} + \frac{1}{z\sqrt{2N+1}}\right) \tag{36}$$

and

$$B = 1/z - 1/y. \tag{37}$$

In the limit $N \to \infty$, one finds

$$U_c = (1+\sqrt{3})\left(\frac{\Delta}{(1+\sqrt{3})/\sqrt{2}} - 1\right)^2. \tag{38}$$

In the particular case of $N = 9$ and $b = 0.1$, where many numerical runs have been performed, (38) becomes

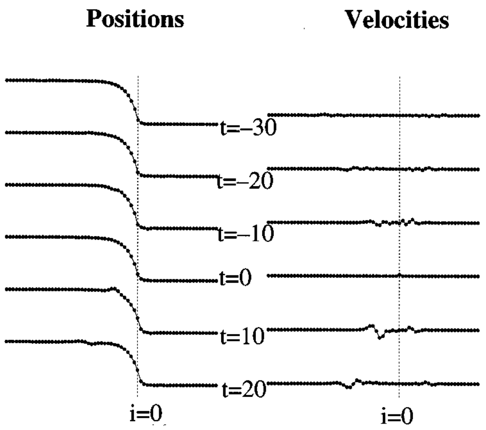

FIG. 4. A creep event obtained from numerical minimization of Eq. (12), for model Eq. (33) with $N = 9$, $\Delta = 1.2$, and $b = 0.1$. Time $t = 0$ is chosen as the instant that the bond at the crack tip snaps. At large negative times the crack is stationary. Traveling waves spontaneously appear far 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.

$$U_c = 0.556(\Delta - 1.663)^2. \tag{39}$$

D. Numerical investigations and jump events

In order to verify Eq. (35), produce pictures of the solutions, and study rapid fracture initiation, I have written numerical routines that directly minimize the functional in Eq. (12) for the model equation (33). The routine requires one to choose a number of particles to study (characteristically 80) and to describe their locations at a number of points in time (characteristically 1500). The complete time history of all particles (characteristically 120 000 variables) is placed into the functional (12), which then is minimized (I used a routine of Press *et al.* [19]) subject to the boundary conditions (11).

Some difficulties came about in attempting to carry out the numerics in such a way that the program would be guaranteed to give a true upper bound to $S[x(t)]$. The finite element method gives such upper bounds, but did not work well in this problem. The reason is that once systems are descending from energy barriers, particles obey Newton's laws (17) and contribute nothing to the functional, as in Eq. (18). Since particles may be moving quite rapidly, there must be very large cancellations in Eq. (12). Finite-element implementations are so insistent upon obtaining a true upper bound that the cancellations cannot be perfect and the numerical answers are so large as to be useless. With a simple finite difference scheme, there exist values for the discretized equations where the cancellation occurs completely and the numerics find these values as part of the solution. The results in Fig. 6 are all from finite-difference and not finite-element calculations.

A numerical solution corresponding to creep appears in Fig. 4. The action of this solution is precisely what is predicted by Eq. (35) and its character is just what is predicted by Eq. (30). The crack begins stationary. Waves enter the system far from the tip and head towards one another, slowly

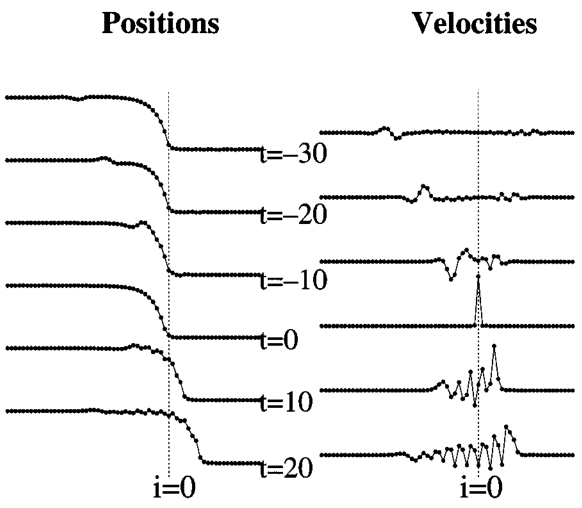

FIG. 5. A jump event obtained from numerical minimization of Eq. (12), for model Eq. (33) with $N=9$, $\Delta=1.2$, and $b=0.1$, precisely the same values as in Fig. 4. However, one now imposes final boundary conditions $\vec{x}$ and $\vec{p}$ corresponding to a running crack and the fluctuations D_i arriving at the crack tip must be larger than in the previous case to achieve them.

growing in amplitude. They strike the tip in perfect synchrony, snapping one bond. The crack tip jumps ahead by one lattice spacing, sending off waves somewhat larger than those that just triggered it, and settles down to a stationary configuration one lattice site to the right of its starting point.

For exactly the same parameter values, a sufficiently large thermal fluctuation can cause a crack to jump to a dynamic configuration. One finds the most likely way for this to occur by solving exactly the same equations used for the creep problem, but by imposing boundary conditions at $t=\tau$ that correspond to a rapidly running crack. Guessing a solution of the form (30) is a reasonable starting point. As initial conditions, I used Eq. (34a), but with the mass at 0 given some large velocity, on the order of 1, and all other mass points motionless. Such states seem to be suitable starting points for numerical hunts for the minimum action, but initially overestimate the minimum action by a factor of more than 2. A solution found in this way appears in Fig. 5. Again, all particles begin at rest, then waves develop far from the crack tip, larger than before, come in towards the center, and drive the crack into action. The kinetic energy of the system increases constantly during the process. Since vanishing of all velocities is a necessary condition for a system to be at a saddle point of the energy, the system cannot be traveling through a traditional saddle point in phase space as it makes the jump to rapid motion.

A plot of the energy U for various values of the driving force Δ appears in Fig. 6. There is a range of Δ for which creep and jump events coexist. Once Δ reaches approximately 1.3, deterministic evolution of the configuration (34a) produces rapidly running, rather than lattice-trapped, cracks. Therefore, for Δ larger than this value, Eq. (35) gives the probability of rapid fracture initiation rather than the rate of creep.

E. Creep rate

Over time periods τ which are long compared to $1/b$, configurations which lead to a single creep event are virtually motionless, except for the brief period when the bond at the origin snaps. The action cannot much depend upon the intermediate time τ_1 at which this happens and therefore the probability of a single creep event occurring in time τ is

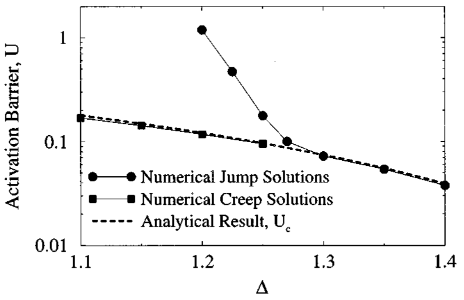

FIG. 6. Results of a numerical search for minimum-energy paths U as a function of Δ. The circles show the activation energy of creep events, the squares show the activation energy of jump events, and the thick line shows a plot of Eq. (39). All the calculations are carried out for $N=9$ and $b=0.1$. At low strains Δ, only creep events are possible. For $\Delta=1.198$ jump events first become possible, although their activation energy 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.

$$\mathcal{P}_1=\Omega\tau e^{-U/kT}. \tag{40}$$

Here Ω is a constant with dimensions of frequency that will be evaluated explicitly in a later section. Similarly, the probability of l creep events occurring is

$$\mathcal{P}_l\sim\frac{(\Omega\tau)^l}{l!}e^{-lU/kT}. \tag{41}$$

The most likely number of creep events to have occurred in this time is given by the maximum of $\mathcal{P}$, which is

$$l=\Omega\tau e^{-U/kT} \tag{42}$$

or

$$\dot{l}=\Omega e^{-U/kT}. \tag{43}$$

Equation (43) accords well with the basic facts on creep rates [1], which show that creep does in fact increase exponentially with temperature; Eqs. (43) and (38) are essentially identical to results of Fuller and Thomson [20].

IV. TIME REVERSAL

A. Antikinetic paths

By considering the limit in which the damping constant b tends to zero, one can make a number of observations concerning the time-reversal invariance of the equations of mechanics. In this limit the spatial scale over which phonons travel without decaying tends to infinity. Therefore, it is possible without noticeable change in any of the solutions of Eq. (3) to set b to zero in a large neighborhood of the crack tip and to mimic a truly Hamiltonian system in contact with an external heat bath. All physical results such as creep rate are perfectly well defined as $b\to 0$, although the formalism becomes indeterminate if b is set to zero at the outset.

In the limit of vanishing damping, one still can speak of a dominant path $\vec{x}(t)$ leading to creep. Focusing upon regions in the neighborhood of the crack tip where the damping has been set to zero, one can watch atoms near the tip evolve in a completely conservative manner. This Hamiltonian trajectory is the path in phase space that has the smallest possible energy leading to creep. Prior to snapping the bond at 0, spatial concentrations of energy become more and more localized in space, until they converge simultaneously upon the crack tip, snapping the bond. After this time, energy disperses throughout the system. Thus even this single Hamiltonian trajectory has characteristics that appear to involve going backward in time initially and then forward in time after the snapping event.

While talk of trajectories moving backward in time appears frivolous, it is an old idea in statistical mechanics. Ehrenfest and Ehrenfest [21] explain Boltzmann's cryptic remark that the H function is everywhere a maximum by considering a system in equilibrium whose H function is found at some times to be at values H_b above the minimum average value and point out that ''in an overwhelming number of cases they form maxima, schematically represented by

$$\begin{array}{ccc} & H_b & \\ H_a & & H_a.\text{''} \end{array} \tag{44}$$

The rise in H is symmetrically related to the fall in H with overwhelming probability. Reflection upon how mechanics might actually implement this symmetry leads to images such as those in Fig. 5. The ''dynamical key'' of Wargitsch and Hubler [22] also provides a case in which time-reversed paths play a crucial role; Wargitsch and Hubler find that the most efficient way to pump energy into a nonlinear system is to force it with the time reverse of the waves it would emit if it were ringing down. Creep fractures progress when thermal fluctuations happen onto the dynamical key for exciting them. Lengthy periods of time-reversed behavior on large scales are impossible, but the underlying symmetry reveals itself during the unlikely progress of activated processes.

B. Time-reversal paradoxes

The apparent conflict between motion-reversal invariance of Newtonian mechanics and the irreversibility of the natural world is a subject that developed with statistical mechanics. It is unlikely that anything could be added now that has not already thoroughly been understood by Boltzmann [23], Ehrenfest and Ehrenfest [21], and Kac [24], or in the books devoted to the topic [25–28]. Nevertheless, the model of fracture studied in this paper provides a revealing case in which to pose again some of the old questions.

Return to the model equation (33), adopt a closed system of finite size, set all dissipative terms b to zero, choose an initial condition in which a crack is present up to some particular point, and ask how this mechanical system will evolve. First, let us consider Loschmidt's objection to Boltzmann; take any Hamiltonian system at any point in time and reverse the sign of the velocities of all particles. Then the system travels backward in time. One can make the paradox worse. According to Liouville's theorem, the volume of phase space associated with any collection of trajectories is unchanged as it undergoes evolution in time. Statistical mechanics promises that the probability of any event depends only upon the phase-space volume of initial conditions that produce it. Since the phase-space volume associated with going backward in time is the same as the volume associated with going forward in time, the two should be equally likely and we should see broken glasses hop off the floor and reassemble themselves on a regular basis.

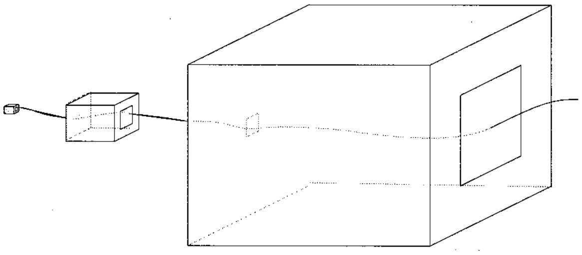

FIG. 7. The progress of a Hamiltonian system through an irreversible process resembles passage through rooms with doors whose sizes increase exponentially. Symmetry of the equations after reversing the sign of time is reflected in the fact that the size of a door is the same whether one passes forwards or backwards through it. Irreversibility comes from the huge new doors that become available.

Boltzmann's answer to Loschmidt is reputed to have been [24] ''go ahead, reverse them!'' The computer seems to make this task possible after all, until one realizes that the task of recording velocities with sufficient precision to reverse them perfectly is computationally intractable except under very limited circumstances [29]. Trying to beat this conjecture, one can put Eq. (33) onto a computer, run it forward in time, and then reverse the velocities. The computer has inevitably lost the exponentially delicate correlations between distant particles needed to make this state effective. The crack runs backward briefly, turns around, and behaves normally. This answer may seem almost as troubling as the original objection because it suggests that when humans are unable to produce or describe a certain initial condition, then nature will be unable to create it. However, one should recognize that systems undergoing irreversible change through fracture are classic branch systems [28], which do not arrive at their initial conditions spontaneously. In laboratory experiments, the initial condition is a result of human action: for example, one takes a notched piece of material and places it under tension. The class of initial conditions that would lead an isolated subsystem to evolve backward in time is inaccessible, both computationally and experimentally.

In addition, consider Eq. (33) with, say, $\Delta=1.2$ and with a small amount of kinetic energy dispersed throughout the system, so that one feels comfortable guessing that the system behaves as if it is at some low temperature and the crack should creep forward. Suppose that at time τ_1 the bond at $i=0$ snaps and the crack moves ahead. It is true that the space of initial conditions that could lead the crack to move backward and heal is just the same size as the space of initial conditions that just made it move forward. However, that is the wrong comparison. The space of initial conditions that could lead the crack to jump over the next bond and progress further is incomparably larger, for the simple reason that the potential energy of the broken bond is now converted to kinetic energy available to aid further snapping events.

Thus we arrive at a schematic description of an irreversible experiment (Fig. 7). A system is prepared in a state far from equilibrium. The preparation process is inevitably asymmetrical in time and cannot incorporate the delicate correlations needed for time-reversed behavior. Following preparation, the system is isolated and begins independent evolution through a sequence of irreversible events. The probability of each of these events happening equals the probability of the event going in reverse. However, each event opens the door to a new event that is vastly more probable.

V. SUBEXPONENTIAL TERMS

A. Path decomposition formula

In order to compute the rate of creep, one must calculate the coefficient Ω that appeared in Eq. (40). There is considerable formal experience with this problem [30,31,8,32], which shows that one needs to look at quadratic fluctuations about the dominant path and compute the determinant of its quadratic form. This task is made difficult by the discontinuities in the force law of Eq. (33). The Taylor expansion of the action is singular at all the critical times where a bond is on the verge of snapping. Fortunately, the path decomposition expansion, due to Auerbach and Kivelson [33], provides a way to write a Green function as an integral over products of Green functions that are restricted to different portions of configuration space. In the case of fracture, the idea will be to write the Green function for a system where a single bond snaps as a product of Green functions, one describing the system before the bond snaps and the other describing it afterward, integrating over the time at which the snap occurs. The Green functions in these two regions can be computed relatively easily since the problems in the two regions are completely linear. This calculation does neglect the contributions from paths in which a bond snaps and reheals many times. There is also another set of approximations adopted having to do with the space of intermediate configurations that in fact leads to a desired final state. Because the solution of these technical problems has been left for the future, I am able to present only an estimate of the prefactors.

Auerbach and Kivelson's decomposition may be generalized as follows: Suppose we divide phase space by a $(2M-1)$-dimensional plane, such as the plane on which some position coordinate reaches the snapping point $x_0^s=1$. If we begin with an ensemble of systems at time $t=0$, then the number of systems that cross this plane during the time interval between t' and dt' and then go on to arrive at a desired final location at time τ is

$$\int dx^s dp^s g_{0\to s}^{t'} dt' \frac{p_0^s}{m} g_{s\to n}^{\tau-t'} \delta(x_0^s-1). \tag{45}$$

The δ function enforces the requirement that each system being considered cross the plane at time t' and the number of systems that cross the plane during dt' is obtained by multiplying by the velocity p_0^s/m. One has to multiply by the probability that the system goes from the crossing point to the desired final state and integrate over all possible crossing points.

Suppose that to get from initial to final states, a system must pass through the plane $x_0^s=1$ at some time. Then one has the identity

$$g_{0\to n}^{\tau}=\int_0^{\tau} dt' \int dx^s dp^s g_{0\to s}^{t'} \frac{p_0^s}{m} g_{s\to n}^{\tau-t'} \delta(x_0^s-1). \tag{46}$$

Despite the fact that Eq. (46) resembles the Chapman-Kolmogorov equation, it is really quite different; the Chapman-Kolmogorov equation says that the probability of going from 0 to n is equal to the probability of going from 0 to s in time t', times the probability of going then on to n, integrated over all intermediate points s. By contrast, Eq. (46) says that the probability of going from 0 to n equals the probability of going from 0 to some particular plane s, which divides 0 from n, times the probability of going from s to n, integrated over the plane, and all times at which one might reach it. It is useful to derive this relation somewhat more formally since it turns out to be possible to generalize it slightly. This task is carried out in Appendix B. The generalization says that the second probability distribution g in Eq. (46) may be replaced by $\bar{g}$, where $\bar{g}$ is a probability distribution appropriate for force $\bar{F}$ rather than F. $\bar{F}$ and F must be equal for $x_0>0$, but on the initial side of this dividing plane, $\bar{F}$ can be chosen arbitrarily.

B. Application to the fracture problem

I now apply this formalism to the crack creep problem. The first task is to decide when creep has occurred. The distribution g gives the probability density of arriving at points in phase space, while a statement such as "the crack moved ahead" is consistent with a broad class of final states. Define the probability of a creep event after time τ as

$$\mathcal{P}=\int dx\ dp\,\theta(x_0)g(\vec{x}\vec{p};\tau). \tag{47}$$

The most likely way for the bond at 0 to snap is for the crack to arrive at, or near, the saddle-point configuration (34a) at some time t'. So long as the momentum of the snapping bond is positive at this time, it is most likely that the crack will progress forward [34]. The estimate embodying this idea is

$$\int dx\ dp\,\theta(x_0)g_{s\to n}^{\tau-t'}\approx\theta(p_0^s). \tag{48}$$

Therefore,

$$\mathcal{P}=\int dt' \int dx^s dp^s \delta(x_0^s-1)\frac{p_0^s}{m} g_{0\to s}^{t'}\theta(p_0^s). \tag{49}$$

Furthermore, for times t' that are large compared to the characteristic time needed for the creep event, $g_{0\to s}^{t'}$ must become independent of t'. Assuming that τ is much larger than this characteristic time, the rate R at which a crack starting in initial configuration 0 makes the transition to the neighborhood of the final configuration is

$$R=\int dx^s dp^s g^{\infty}_{0\rightarrow s}\delta(x_0^s-1)\frac{p_0^s}{m}\theta(p_0^s). \tag{50}$$

The probability of starting at rest and arriving near a configuration with a bond about to snap is given by Eq. (28) and is proportional to $\exp[-E(\vec{x}^s,\vec{p}^s)/k_BT]$. Thus one may rewrite Eq. (50) as [35]

$$R=\frac{\displaystyle\int dx^s dp^s e^{-E(\vec{x}^s,\vec{p}^s)/k_BT}\delta(x_0^s-1)\frac{p_0^s}{m}\theta(p_0^s)}{\displaystyle\int dx^s dp^s e^{-E(\vec{x}^s,\vec{p}^s)/k_BT}}. \tag{51}$$

The energy is quadratic in momenta, so one can do the momentum integrals, obtaining an expression depending upon the potential energy V as

$$R=\sqrt{\frac{k_BT}{2\pi m}}\frac{\displaystyle\int dx^s e^{-V(\vec{x}^s)/k_BT}\delta(x_0^s-1)}{\displaystyle\int dx^s e^{-V(\vec{x}^s)/k_BT}}. \tag{52}$$

We have already identified U_c as the minimum-energy configuration at which x_0^s has been taken to the snapping point. Holding the bond at 0 fixed, the energy is just a quadratic functional of all remaining variables, unless a neighboring bond moves far enough to snap as well. Ignoring these very large excursions, there is a unique matrix V'' that describes quadratic energy fluctuations. Thus, shifting the integration coordinates to the appropriate minimum configuration, dropping the superscript s, and expanding V gives

$$R=\sqrt{\frac{k_BT}{2\pi m}}e^{-U_c/k_BT}\frac{\displaystyle\int dx\ \exp\left(-\sum_{i,j} x_iV_{ij}''x_j/k_BT\right)\delta(x_0)}{\displaystyle\int d^Mx\ \exp\left(-\sum_{ij} x_iV_{ij}''x_j/k_BT\right)}, \tag{53}$$

$$=\sqrt{\frac{k_BT}{2\pi m}}e^{-U_c/k_BT}\times\frac{\displaystyle\int dx\int\frac{dz}{2\pi}e^{izx_0}\exp\left(-\sum_{i,j} x_iV_{ij}''x_j/k_BT\right)}{\displaystyle\int dx\ \exp\left(-\sum_{i,j} x_iV_{ij}''x_j/k_BT\right)}, \tag{54}$$

$$=\sqrt{\frac{k_BT}{2\pi m}}e^{-U_c/k_BT}\int\frac{dz}{2\pi}e^{-z^2k_BTG_{00}/4}, \tag{55}$$

$$=\sqrt{\frac{1}{2\pi^2 m}}e^{-U_c/k_BT}\frac{1}{\sqrt{G_{00}}}, \tag{56}$$

where the matrix G_{ij} is the inverse of V''.

Computation of G_{00} is simplest for the model defined by Eq. (33) in the limit $N\rightarrow\infty$. One finds

$$G_{00}=\frac{\sqrt{3}-1}{2}, \tag{57}$$

giving a final result

$$R=\frac{1}{\pi}\sqrt{\frac{1}{(\sqrt{3}-1)}}\ e^{-U_c/k_BT}. \tag{58}$$

The original model had a number of dimensional constants set to unity. If all the springs in the model had constant K and if all the masses were m, then R would be proportional to $\omega=\sqrt{K/m}$.

Computation of the prefactor for the jump problem proceeds in an identical fashion, although uncertainties related to the precise set of intermediate configurations that leads to the desired final running state are more severe. Let p_0^s be the momentum of the bond at 0 at the instant it snaps. Using as the analog of Eq. (48) the assumption that all configurations with momentum $p_0>p_0^s$ will likewise proceed to the running state, one finds exactly the same expression as Eq. (58), but multiplied by an additional factor of

$$\sqrt{\frac{kT}{\pi(p_0^s)^2/2m}}. \tag{59}$$

VI. CONCLUSIONS

Since there is substantial literature on creep fracture [1], including careful experiments, it would be natural to conclude this paper with an attempt at quantitative comparison. Instead, I must conclude by explaining why the comparison is not yet possible.

There is first the difficulty that quantum-mechanical fluctuations compete with thermal fluctuations in providing a mechanism for atoms to cross energy barriers. The characteristic temperature below which the quantum-mechanical influence upon lattice vibrations cannot be neglected is the Debye temperature, which is on the order of room temperature (see Ref. [36], p. 461). Simple estimates carried out by Gilman and Tong [6] show that the effects are not small.

There is second the difficulty that creep fracture is enormously influenced by chemical reactions at the fracture tip, which change the speed of creep by orders of magnitude [13]. For example, moisture has such an effect upon cracks in glass.

There is third the difficulty that one- and two-dimensional models do not capture the right geometry by which creep fracture must proceed. In three dimensions, the crack line advances by forming tiny bumps, which reach out ahead of the main crack [6]. Below a critical size they will shrink and above it they will grow. One interpretation of the one-dimensional model discussed in this paper is that it describes part of one of these structures along a crack line in three dimensions. Even in two dimensions crack tips can become blunted, which means that there are many metastable configurations of atoms near the crack tip that have large effects upon its ability to propagate.

When one passes from the creep problem to the jump problem, the comparison with experiment becomes even more tenuous. The phenomenon of static fatigue sounds intriguing; an experimental sample is placed under a static load and one waits until it fractures. However, in checking the experimental literature, I have not found a case in which the comparison is really appropriate. In characteristic experiments [37,38], cracks are placed in loading conditions where as they creep ahead, the energy flowing to their tips increases for reasons associated with the loading geometry. The experiments measure creep combined with a geometrical instability, rather than the jump phenomenon I have been describing theoretically. Therefore, at the end of this investigation, the tasks still to be accomplished seem more numerous than those that have been completed.

ACKNOWLEDGMENTS

Robert S. Maier has patiently explained to me why results for prefactors, which I had hoped were exact, in fact are crude approximations, and several astute remarks from J. S. Langer have led me to revise portions of the manuscript. I have had financial support from the Alcoa Foundation, the Exxon Educational Foundation, the U.S.–Israel Binational Science Foundation (Grant No. 920-00148/1), the Texas Advanced Research Program, and the National Science Foundation (Grant No. DMR-9531187).

APPENDIX A: DERIVATION OF FUNCTIONAL INTEGRAL

Starting from Eq. (3), one may write

$$g(\vec{x}\vec{p};\tau+dt)=\prod_i\left[1+\left(-\frac{\partial}{\partial x_i}\frac{p_i}{m}+\frac{\partial}{\partial p_i}\left\{-F_i+bp_i+mkTb\frac{\partial}{\partial p_i}\right\}\right)dt\right]g(\vec{x}\vec{p};\tau) \tag{A1}$$

and then insert the complete set of states

$$\int\left\{\prod_i\frac{dx_i'dp_i'dk_i^xdk_i^p}{(2\pi)^2}e^{ik^x(x_i'-x_i)+ik_i^p(p_i'-p_i)}\left[1+\left(-\frac{\partial}{\partial x_i'}\frac{p_i'}{m}+\frac{\partial}{\partial p_i'}\left\{-F_i+bp_i'+mkTb\frac{\partial}{\partial p_i'}\right\}\right)dt\right]\right\}g(\vec{x}'\vec{p}';\tau) \tag{A2}$$

$$=\int\left\{\prod_i\frac{dx_i'dp_i'dk_i^xdk_i^p}{(2\pi)^2}e^{ik^x(x_i'-x_i)+ik_i^p(p_i'-p_i)}\left[1+\left(ik_i^x\frac{p_i'}{m}-ik_i^p\{-F_i+bp_i'-ik_i^pmkTb\}\right)dt\right]\right\}g(\vec{x}'\vec{p}';\tau) \tag{A3}$$

$$\approx\int\left\{\prod_i\frac{dx_i'dp_i'dk_i^xdk_i^p}{(2\pi)^2}e^{ik^x(x_i'-x_i)+ik_i^p(p_i'-p_i)}e^{[ik_i^x(p_i'/m)-ik_i^p\{-F_i+bp_i'-ik_i^pmkTb\}]dt}\right\}g(\vec{x}'\vec{p}';\tau) \tag{A4}$$

$$=\int\left\{\prod_i\frac{dx_i'dp_i'dk_i^p}{2\pi}\delta(x_i'-x_i+dt\ p_i'/m)e^{ik_i^p(p_i'-p_i)}e^{[-ik_i^p\{-F_i+bp_i'\}-(k_i^p)^2mkTb]dt}\right\}g(\vec{x}'\vec{p}';\tau) \tag{A5}$$

$$=\int\left\{\prod_i\frac{dx_i'dp_i'}{2\pi}\delta(x_i'-x_i+dtp_i'/m)\sqrt{\frac{\pi}{mkTbdt}}e^{\frac{-[p_i'-p_i+dt(F_i-bp_i')]^2}{4mkTbdt}}\right\}g(\vec{x}'\vec{p}';\tau). \tag{A6}$$

With a slight change in notation, (A6) becomes (5).

APPENDIX B: FORMAL DERIVATION OF DECOMPOSITION FORMULA

This method is based on the procedure of van Baal [39], but requires some generalization. There are three steps. First, one finds a partial differential equation for g in terms of the initial positions and momenta of the particles rather than final positions and momenta. Second, one broadens the equation to a wide class of force laws. Third, one takes the Laplace transforms of the two differential equations, and by multiplying them by appropriate factors of g, subtracting two equations, and using the Laplace convolution theorem gets Eq. (46).

Step I. One can rewrite the probability to go from initial to final states as

$$g_{0\to n}^{\tau}=\int dx^s\int dp^sg_{0\to s}^{dt}g_{s\to n}^{\tau-dt}. \tag{B1}$$

From the Fokker-Planck equation (3) one has that

$$g_{0\to s}^{dt}=\left[1-\sum_i\frac{\partial}{\partial x_i^s}\frac{p_i^s}{m}+\frac{\partial}{\partial p_i^s}\left\{-F_i+bp_i^s+mkTb\frac{\partial}{\partial p_i^s}\right\}\right]\delta(x^s-x^i)\,\delta(p^s-p^0). \tag{B2}$$

Placing Eq. (B2) into (B1) and integrating by parts to remove the differential operators from the δ functions gives immediately

$$\frac{\partial g}{\partial t}=\sum_i\left[\frac{p^0}{m}\frac{\partial}{\partial x_i^0}+[F_i(x^0)-bp_i^0]\frac{\partial}{\partial p_i^0}+mbk_BT\frac{\partial^2}{p_i^{02}}\right]g. \tag{B3}$$

This equation relates the evolution of the probability of starting at initial condition 0 and ending at final condition n to derivatives of the function with respect to the initial conditions. The operator acting upon g is the adjoint of the operator in (3).

Step II. Consider a probability distribution $\overline{g}$. This distribution obeys exactly the equations as g, except that the force function F appearing in Eq. (B3) is replaced by $\overline{F}$, where $\overline{F}$ is any function that is identical to F for $x_0>0$ and can be anything whatsoever for $x_0<0$. It might equal F there too, or it might be $-\infty$, in which case it represents an infinite cliff swallowing up any particle whose coordinate passes the plane $x_0=0$. In the first case g and $\overline{g}$ are the same, while in the latter case $\overline{g}$ is a probability distribution that vanishes for $x_0^0<0$. The equation obeyed by $\overline{g}$ is

$$\frac{\partial\overline{g}}{\partial t}=\sum_i\left[\frac{p^0}{m}\frac{\partial}{\partial x_i^0}+[\overline{F}_i(x^0)-bp_i^0]\frac{\partial}{\partial p_i^0}+mbk_BT\frac{\partial^2}{p_i^{02}},\right]\overline{g}. \tag{B4}$$

Step III. Take the Laplace transform of Eqs. (3) and (B4). One has

$$\delta(x^s-x^0)\,\delta(p^s-p^0)+\left\{-E+\sum_i\left[-\frac{\partial}{\partial x_i^s}\frac{p_i^s}{m}-\frac{\partial}{\partial p_i^s}\{F_i-bp_i^s\}+mkTb\frac{\partial^2}{p_i^{s2}},\right]\right\}g_{0\to s}^E, \tag{B5}$$

$$\delta(x^s-x^n)\,\delta(p^s-p^n)+\left\{-E+\sum_i\left[\frac{\partial}{\partial x_i^s}\frac{p_i^s}{m}+\{F_i-bp_i^s\}\frac{\partial}{\partial p_i^s}+mkTb\frac{\partial}{p_i^{s2}}\right]\right\}\overline{g_{s\to n}^E}. \tag{B6}$$

Multiply Eq. (B5) by $\theta(x_0^s)\overline{g_{s\to n}^E}$, multiply Eq. (B6) by $\theta(x_0^s)g_{0\to s}^E$, subtract the two equations, and integrate over x^s and p^s. The terms involving derivatives with respect to p^s turn into perfect differentials of products of the functions g and $\overline{g}$ and vanish, as do derivatives with respect with all components of x^s except x_0^s. What remains is

$$\theta(x_0^n)g_{0\to n}^E=\int dx^s dp^s\,\delta(x_0^s)\frac{p_0^s}{m}g_{0\to s}^E g_{s\to n}^E. \tag{B7}$$

Inverting the Laplace transform, using the convolution theorem, Eq. (B7) produces Eq. (46).

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[1] H. E. Evans, *Mechanisms of Creep Fracture* (Elsevier, London, 1984).

[2] T. A. Michalske, W. L. Smith, and J. E. Houston, J. Appl. Phys. **76**, 2109 (1994), come close to a realization of the experiment described here.

[3] H. A. Kramers, Physica **7**, 284 (1940).

[4] N. G. van Kampen, *Stochastic Processes in Physics and Chemistry* (North-Holland, Amsterdam, 1992).

[5] P. Hänggi, P. Talkner, and M. Borkovec, Rev. Mod. Phys. **62**, 251 (1990).

[6] J. J. Gilman and H. C. Tong, J. Appl. Phys. **42**, 3479 (1971).

[7] R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).

[8] L. Schulman, *Techniques and Applications in Path Integration* (Wiley, New York, 1981).

[9] M. F. Kanninen and C. Popelar, *Advanced Fracture Mechanics* (Oxford University Press, New York, 1985).

[10] A. A. Griffith, Philos. Trans. R. Soc. London Ser. A **221**, 163 (1921).

[11] R. Thomson, C. Hsieh, and V. Rana, J. Appl. Phys. **42**, 3154 (1971).

[12] R. Thomson, Solid State Phys. **39**, 1 (1986).

[13] B. Lawn, *Fracture of Brittle Solids*, 2nd ed. (Cambridge University Press, New York, 1993).

[14] L. I. Slepyan, Sov. Phys. Dok. **26**, 538 (1981).

[15] S. A. Kulakhmetova, V. A. Saraikin, and L. I. Slepyan, Mech. Solids **19**, 101 (1984).

[16] M. Marder and X. Liu, Phys. Rev. Lett. **74**, 2417 (1993).

[17] M. Marder and S. Gross, J. Mech. Phys. Solids **43**, 1 (1995).

[18] M. Marder, Physica D **66**, 125 (1993).

[19] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in C*, 2nd ed. (Cambridge University Press, Cambridge, 1992).

[20] E. R. Fuller and R. Thomson, in *Fracture Mechanics of Ceramics*, edited by R. C. Bradt, D. P. H. Hasselman, and F. F. Lange (Plenum, New York, 1978), Vol. 4, pp. 507–548.

[21] P. Ehrenfest and T. Ehrenfest, *The Conceptual Foundations of the Statistical Approach in Mechanics* (Cornell University Press, Ithaca, 1959).

[22] C. Wargitsch and A. Hubler, Phys. Rev. E **51**, 1508 (1995).

[23] L. Boltzmann, *Lectures on Gas Theory* (University of California Press, Berkeley, 1964).

[24] M. Kac, *Probability and Related Topics in Physical Science* (Interscience, London, 1959), Chap. III, particularly p. 78.

[25] *Physical Origins of Time Asymmetry*, edited by J. J. Halliwell, J. Perez-Mercader, and W. H. Zurek (Cambridge University Press, Cambridge, 1994).

[26] H. J. Kreuzer, *Nonequilibrium Thermodynamics and its Statistical Foundations* (Clarendon, Oxford, 1981).

[27] P. C. W. Davies, *The Physics of Time Asymmetry* (University of California Press, Berkeley, 1977).

[28] H. Riechenbach, *The Direction of Time* (University of California Press, Berkeley, 1956).

[29] Many statements in this section are implicitly based upon the assertion that the model system studied in this paper has a positive Lyapunov exponent. This assertion is not easy to check and is not obviously true since the forces between mass points are almost always linear. One can view the model as a map in which an initial condition is decomposed into normal modes and evolves according to linear transformations in between bond snapping events. Clearly, given two systems that differ by some slight fixed amount in initial conditions, there exist cases such that one of them would snap a bond at some time and the other would not. I have not analyzed how often

these cases would occur; they are sufficiently rare as to be hard to pick up numerically.

[30] R. L. Stratonovich, *Topics in the Theory of Random Noise* (Gordon and Breach, New York, 1963), Vol. 1.

[31] J. S. Langer, Ann. Phys. (N.Y.) **41**, 108 (1967).

[32] M. Büttiker and R. Landauer, in *Nonlinear Phenomena at Phase Transitions and Instabilities*, edited by T. Riste (Plenum, New York, 1982), pp. 111–143.

[33] A. Auerbach and S. Kivelson, Nucl. Phys. **B257**, 799 (1985).

[34] Transition-state theory assumes that systems do not cross energy barriers multiple times and needs to be corrected when this assumption fails. Determining precisely the set of particle positions and momenta that causes the creep event to go forward, once given that the bond at 0 has reached the snapping point, is an extremely elaborate problem in classical mechanics. For example, if the neighbors of mass 0 have sufficiently large negative momentum, they will force the bond at 0 to heal almost immediately. The effort that would be required to deal with this complication accurately does not seem worthwhile in view of the small changes expected in the prefactor.

[35] Paths involving multiple snapping and rehealing of the bond are being neglected at this juncture.

[36] N. Ashcroft and N. D. Mermin, *Solid State Physics* (Saunders, Fort Worth, 1976).

[37] M. K. Ferber and P. F. Becher, J. Am. Ceram. Soc. **73**, 2038 (1990).

[38] M. J. Jatthewson and C. R. Kurkjian, J. Am. Ceram. Soc. **70**, 662 (1987).

[39] P. van Baal, in *Lectures on Path Integration*, edited by H. A. Cerdeira *et al.* (World Scientific, Singapore, 1993), pp. 54–83.