Monte Carlo dynamics of driven elastic strings in disordered media

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We show that the common local Monte Carlo rules used to simulate the motion of driven elastic strings in disordered media cannot capture the interplay between elasticity and disorder which lies at the heart of these systems. We therefore discuss a class of generalized Monte Carlo algorithms where an arbitrary number of line elements may move at the same time. We prove that all these dynamical rules have the same value of the critical force and possess phase spaces made up of a single ergodic component. A variant Monte Carlo algorithm allows us to compute the critical force of a sample in a single pass through the system. We establish dynamical scaling properties and obtain precise values for the critical force, which is finite even for an unbounded distribution of the disorder. Extensions to higher dimensions are outlined.

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In the last few years, the study of elastic manifolds in random media has received much attention.

These systems appear in a wide range of physical systems, ranging from vortices in type-II superconductors[1] to charge density waves,[2] to interfaces in disordered magnets,[3] and to the problem of directed polymer growth.[4] The response of elastic manifolds to an external driving force f is highly nontrivial: at temperature $T=0$, the manifold is completely ''pinned'' at small forces, while it moves with nonzero velocity at forces larger than a certain critical force f_c. At finite, but small, T, a so-called ''creep motion'' takes place for $f \ll f_c$, while the motion at $f \gg f_c$ is described by viscous flow. Many details of this dynamical problem, both at $T=0$ and at finite temperatures, have yet to be understood fully.[5,6]

This paper is concerned with an analysis of the dynamical Monte Carlo method[7] as applied to lattice models of driven elastic manifolds in random media. We argue that the common local Monte Carlo rules[8–11] are often incompatible with the Langevin dynamics,[12–14] which defines time evolution in continuum models. We instead propose generalized Monte Carlo algorithms where an arbitrary number of elements may move at the same time. For this class of algorithms, we can establish the uniqueness of the critical force and single connectedness of phase space. Furthermore, we devise a method which simplifies enormously the calculation of the critical force.

Our model is sketched in Fig. 1. We consider a one-dimensional manifold, an elastic string, $x^t=\{x_i^t\}_{i=0,\ldots,L}$, moving at times $t=0,1,2,\ldots$ on a spatial square lattice with a random potential $V(i,x)$ with $x=0,1,\ldots$. We also introduce a metric constraint

$$|x_{i+1}^t - x_i^t| \leqslant 1 \tag{1}$$

as well as periodic boundary conditions ($x_0^t=x_L^t$) on the string. The random potential satisfies

$$V(i,x_i+M)=V(i+L,x_i)=V(i,x_i). \tag{2}$$

This condition defines an effective sample of size (L,M). While Eq. (2) is important for the following, the periodic boundary condition for the string and the specific choice of lattice are inessential details.

The energy of an elastic string x^t in the presence of an external driving force f is given by

$$E(x^t)=\sum_{i=1}^{L} V(i,x_i^t) - f x_i^t + E_{el}(|x_{i+1}-x_i|). \tag{3}$$

The last term in Eq. (3) is the elastic energy E_{el}. The algorithm presented in this paper remains valid as long as $E_{el}(|x_{i+1}-x_i|)$ is convex and with a general random potential.

In Fig. 1, a local Monte Carlo move is indicated. In the local Monte Carlo algorithm, the proposed configuration $\tilde{x}$ differs from the present configuration x^t only on a random position i. One chooses $\tilde{x}_i = x_i \pm 1$ with equal probability. At zero temperature, the move is accepted ($x^{t+1}=\tilde{x}$) if the energy, Eq. (3), decreases and if the metric constraint, Eq. (1), is satisfied. Otherwise, it is rejected ($x^{t+1}=x^t$).

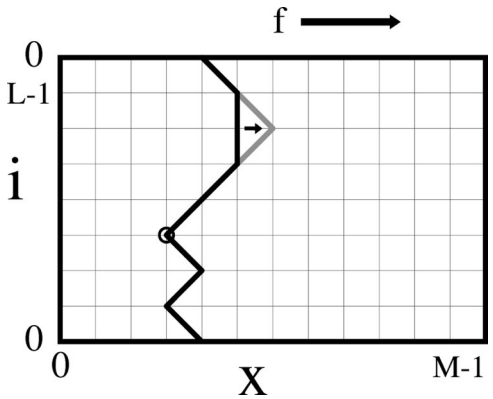

FIG. 1. Elastic string $x^t=\{x_i^t\}_{i=0,\ldots,L}$ on a spatial square lattice with disorder potential $V(i,x)$. Periodic boundary conditions in i and x are assumed for the lattice and the disorder, respectively. The direction of the driving force f is indicated, as well as a proposed *local* Monte Carlo move. The local dynamics leads to a trivial critical force in the limit of large systems.

This rule has been used in past simulations, in spite of its very serious shortcomings. Consider, for example, the site in Fig. 1 marked with a circle, (i_0,x_0). The string x^t shown in Fig. 1 can only move away from (i_0,x_0) if $f>V(i_0,x_0+1)-V(i_0,x_0)+c$. Even an infinitely long string $(L\to\infty)$ is thus stopped by a single deep pin $V(i_0,x_0)$ and the motion does not differ qualitatively from the one of a point in a disordered potential.[15,16] For an unbounded distribution of V, the critical force is infinite. Notice that f is a force *density*. The local Monte Carlo algorithm generates the inconsistent feature that in order to liberate a long flux line from a single deep pin we have to apply an infinite driving force on any single point on the line. The scenario which we just discussed for the metric constraint remains unchanged for any elastic potential stronger than the harmonic one [e.g., $E_{el}=c_1(x_{i+1}-x_i)^2+c_2(x_{i+1}-x_i)^4$]. Only for an at most harmonic elastic potential may the local Monte Carlo algorithm overcome a single deep pin. In that case, we find on the lattice a critical force for the local Monte Carlo algorithm which differs from the one obtained with our more general algorithm.

Some authors have countered the mentioned difficulties by using a bounded distribution, $|V|<V_{\max}$. In this case, the critical force of the local Monte Carlo algorithm will be trivially $f_c=2V_{\max}$ and, as already pointed out for the random Ising model,[9] the dynamics of the string will be similar to the motion of the nondisordered system.

We conclude that the description of a driven elastic string by means of a local Monte Carlo algorithm or its variants[11] eliminates the very feature which makes the problem interesting in the first place: namely, the competition between elasticity and disorder. This competition is preserved in the continuum Langevin dynamics.[13,5]

Within the Monte Carlo method, we are thus naturally lead to consider generalizations of the model. The only option is to abandon the local moves in favor of rules which allow extended moves. The study of extended moves in dynamical Monte Carlo is the subject of this paper. Let us note from the beginning that in the continuum Langevin dynamics the energy is local, but that the *gradient* of the energy $\nabla E=-dx^t/dt$ is an L-component vector which will correspond to an extended move in our Monte Carlo approach. The above argument shows that, on a lattice for the cases considered, we cannot consistently decompose gradient motion into a succession of single-component moves.

Let us define "model *a*" dynamics by a proposed move $x^t\to x^t+\delta^t$ with $\delta^t=\{\delta_i^t\}_{i=0,\ldots,L}$ such that

$$\delta_i^t=\left\{\begin{array}{ll} +1 & p \\ 0 \quad \text{with prob.} & 1-2p \\ -1 & p \end{array}\right\}\ \forall i \quad (\text{model } a). \qquad (4)$$

At zero temperature, the proposed move is accepted, $x^{t+1}=x^t+\delta^t$, if the resulting configuration both satisfies the metric constraint, Eq. (1), and decreases the string energy, Eq. (3). Note that under model *a* dynamics a move is proposed with the same probability as its inverse. This serves to enforce detailed balance, which allows us to naturally generalize the rule to finite temperatures via the Metropolis algorithm. The same can usually not be done for cellular automata methods.[13,14,17]

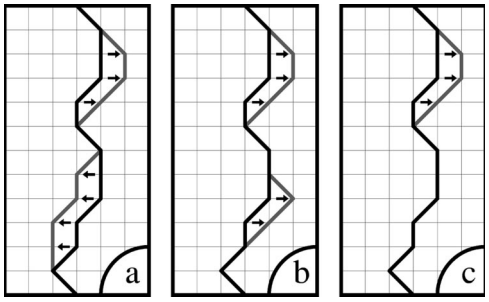

FIG. 2. Nonlocal Monte Carlo moves which are considered in this paper. Model *a*: *all* positions x_i^t $(i=1,\ldots,L)$ may change at the same time by a value ±1. Model *b*: as in *a*, but the motion is either in forward or in backward direction. Model *c*: as in *b*, but the motion is restricted to single "fronts."

A possible second rule ("model *b*") chooses at each time t with equal probability either to move forward $(\mu^t=1)$ or backwards $(\mu^t=-1)$. The following move is then proposed:

$$\delta_i=\left\{\begin{array}{ll} \mu^t & p \\ \quad \text{with prob.} & \\ 0 & 1-p \end{array}\right\}\ \forall i \quad (\text{model } b). \qquad (5)$$

The simulation of dynamical models with such global moves may appear hopeless because of the difficulty to detect the few energetically favorable choices among the exponential number of possibilities in Eq. (4) or in Eq. (5).

To show that the situation is much less desperate, let us first define a "forward front" of length k as a contiguous set of points $i,i+1,\ldots,i+k-1$, which may advance together without violating the metric constraints, Eq. (1) $(\delta_i=\delta_{i+1}\ldots=\delta_{i+k-1}=1$ with $\delta_{i-1}\neq1,\ \delta_{i+k}\neq1)$. A "backward front" is defined analogously. We call "unstable" a front which lowers the energy, Eq. (3). The moves proposed in Figs. 2(a) and 2(b) each consist of *two* fronts. At least one of these must be unstable if the move is to be accepted (this is immediately apparent for model *b* and follows for model *a* from an elementary consideration). To determine whether a configuration x^t is unstable, we only need to consider the at most $2L(L-1)+2$ fronts of x^t rather than the exponential number of moves in Eq. (4) or Eq. (5).

Besides model *a* and model *b* dynamics, it is also possible to set up single-front dynamical rules which respect detailed balance. These rules [as sketched in Fig. 2 (c)] can be simulated with less effort than model *a* or model *b*. Even in the latter cases, though, we have developed methods which realize Eqs. (4) and (5) while never attempting a move forbidden by Eq. (1).

Our main point in the present paper is that a great deal of information is available without actually simulating the dynamic rules. We will show that f_c is the same for all models and that the critical string can be obtained easily.

We define, for an arbitrary string x^α, the "depinning force" $f_d(x^\alpha)$ as the smallest non-negative f in Eq. (3) which

destabilizes one forward front. Furthermore, we define the critical force of a given sample (of size $L\times M$) as

$$f_c=\max_{\{x^\alpha\}} f_d(x^\alpha), \tag{6}$$

where $\{x^\alpha\}$ is the set of all possible strings. Notice that the definiton of f_c or $f_d(x^\alpha)$ is model independent. We show in the following that f_c in Eq. (6) is an appropriate definition for all cases as, for a driving force $f<f_c$, the system will be pinned in the long-time limit $t\to\infty$.

To prove the above, we introduce a variant Monte Carlo (VMC) algorithm which, as a by-product, will allow us to actually compute f_c with great ease.

At each time step $t=0,1,\ldots$, the VMC algorithm simply moves a single front of *minimal* length k among the unstable forward and backward fronts. The VMC method violates detailed balance and is not a valid Monte Carlo algorithm as it stands. However, each move possible within the VMC algorithm is also allowed with all the other models considered.

We have proved the following theorem: if, under VMC dynamics at driving force f, a string x^α is pinned in the forward direction, it can at most recede towards a configuration x^β ($x_i^\beta\leqslant x_i^\alpha\forall i$), which is itself pinned in the forward direction. Eventually, we will reach a string x^γ which is pinned in the both forward and backward directions. This string x^γ is pinned for all models; if it is pinned at f_c, we call it a ''critical elastic string'' x^c. The theorem can be easily proved for a general elastic energy, which is local and convex, by taking into account that the VMC algorithm only moves fronts of minimal size.

The theorem allows us to understand that Eq. (6) is indeed an appropriate definition for all models: As we defined $f_d(x^\alpha)$ only with respect to *forward* motion, one might have imagined that a string which cannot advance at f_c could move backwards and then be avoided during the subsequent forward evolution. Our theorem tells us that such loopholes do not exist: Under VMC dynamics, an elastic string which can no longer move forward, will move backwards and then stop.

Conversely, we can show that a string which can no longer move backwards under the VMC dynamics will exclusively move forward and then stop. This observation simplifies the numerical computations of the VMC algorithm.

Now, we show how to actually determine f_c and x^c. There is no guarantee that a generic dynamic rule (such as model *a* or model *b*) will actually stop at x^c, when driven at forces $f\leqslant f_c$. We performed simulations in small systems, where f_c and x_c could be obtained by exact enumeration, and observed that the string could pass the periodic sample many times without getting pinned. We initially even suspected that x^c could be dynamically inaccessible from part of phase space.

In this context, we were able to prove a second theorem: Starting at an initial configuration x^{t_0} with $x_i^{t_0}\leqslant x_i^c$, the VMC algorithm at driving force $f\leqslant f_c$ can never pass x^c (cf. Ref. 18 for a related ''no-passing'' theorem for continuum Langevin motion).

In practice, we simply update the driving force by the present depinning force $f=f_d(x^t)$ each time we get stuck at a configuration x^t. In one pass through the system, we will have obtained the critical force. The computation of f_c and of the critical string is thus extremely simple.

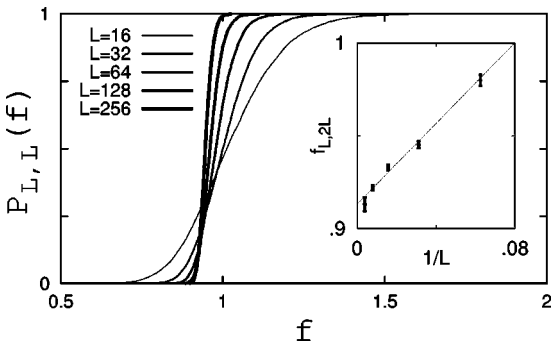

FIG. 3. Main figure: probability $P_{L,L}(f)$ to have a critical force $f_c<f$ vs f for samples of size (L,L) vs L for $L=16,32,\ldots,512$. The elastic constant is $c/2=1$, and a Gaussian normal distribution is used for the disorder potential. For all large M, the curves $P_{L,M}(f)$ and $P_{2L,2M}(f)$ intersect at the same force, $f_{L,2L}$ which, in the inset, is plotted vs $1/L$. The extrapolated value of $f_{L,2L}$ in the limit $1/L\to 0$ is the critical force f_c^∞ of a macroscopic sample.

Furthermore, the VMC algorithm gives an explicit construction—for any of the methods—which dynamically connects an arbitrary initial state with a critical string. This proves that all the models in Fig. 2 possess a single ergodic component.

We now present our numerical calculations which show that f_c is finite for a sample of size (L,M) in the limit $L,M\to\infty$ with $L/M=\text{const}$. In all our calculations, we have used a Gaussian normal distribution for the random potential.

For finite sizes (L,M), we define the integrated distribution function $P_{L,M}(f)$ as the probability that a sample of size (L,M) possesses a critical force $f_c\leqslant f$. Because of the metric constraint, Eq. (1), we know that the lateral extension of the string, $\max_{i,j}|x_i-x_j|$, will be at most $L/2$. This can be used to show that for $M\gg L/2$

$$P_{L,2M}(f)=P_{L,M}^2(f). \tag{7}$$

We will be interested in the intersection point $f_{L,2L}$ between the integrated probability distribution for the system of size (L,M) and the one of size $(2L,2M)$:

$$P_{L,M}(f_{L,2L})=P_{2L,2M}(f_{L,2L}). \tag{8}$$

In fact, the single intersection $f_{L,2L}$ will not depend on M for large M, by virtue of Eq. (7). In our opinion, this observation implies that the natural scaling for our system in the thermodynamic limit is $M\sim L^\gamma$ with $\gamma=1$, i.e., that we should compare the system of size (L,M) with another one, double in size both in L and in M.

We have checked numerically that corrections to the scaling relation, Eq. (7), are already negligible for $L\sim M$ (for $L>4$) and that intersection points $f_{L,2L}$ indeed do not depend on $M>L$. In Fig. 3 we show data for $P_{L,L}(f)$ for $L=16,32,\ldots,512$. The inset of the figure gives the $f_{L,2L}$ as a function of $1/L$ for all sizes. It is evident that $f_{L,2L}$ extrapolates to a finite value, the critical force of the model in the

thermodynamic limit, f_c^∞. We find $f_{L,2L} \to f_c^\infty = 0.91 \pm 0.01$ for $c/2 = 1$. The numerical value of f_c^∞ is due in part to the value of c and to the imposed constraint. We stress again that f_c^∞ is independent of the aspect ratio L/M.

The study of the statistical properties of the critical string x_c goes beyond the scope of this paper.[19] We simply point out here that the size k of the minimal unstable front is distributed approximately as $p(k) \sim \exp(-k/k_{typ})$ (for large k). Here, k_{typ} depends on the elasticity parameter c, but remains finite as $L \to \infty$, although the VMC algorithm authorizes fronts of all sizes.

Finally, we discuss possible extensions of the work presented here. We already indicated that our metric constraint was introduced mainly for convenience as our theorems and the VMC algorithm remain valid if E_{el} is a general convex function. In the absence of the constraint, the lateral extension of the string may however scale as L^γ with $\gamma > 1$. If so, our scaling assumption, Eq. (7), would have to be modified. We have also extended most of our results to higher-dimensional manifolds and embedding spaces. There, the only critical issue seems to be the complexity of the VMC algorithm, as the number of possible fronts can be much larger than in the linear string.

In conclusion, we have put the dynamical Monte Carlo algorithm for the motion of elastic manifolds in random media on a solid footing. We have shown that only extended-move schemes can capture the subtle interplay between elasticity and disorder, which is totally absent from the customary local algorithms. Our theorems allowed us to compute features universal to all members of this class: namely, the critical force, as well as properties of the critical string. The variant Monte Carlo algorithm is crucial in that it allows us to compute the critical force with full rigor even for samples which are several orders of magnitude larger than those accessible to exact enumeration methods. In the continuum, the Langevin dynamics also satisfies a ''no-passing'' condition,[18] which has so far not allowed the rigorous computation of critical elastic strings, as the numerical discretizations have to be controlled. Our dynamical Monte Carlo approach can be thought of as a rigorous cellular automaton model which is consistent with the continuum models. Furthermore, it implements the basic concept of detailed balance and is therefore much easier to generalize to finite temperatures than previous continuum and lattice formulations.

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