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Variant Monte Carlo algorithm for driven elastic strings in random media

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Abstract

We discuss the non-local 'Variant Monte Carlo' algorithm which has been successfully employed in the study of driven elastic strings in disordered media at the depinning threshold. Here we prove two theorems, which establish that the algorithm satisfies the crucial 'no-passing' rule and that, after some initial time, the string exclusively moves forward. The Variant Monte Carlo algorithm overcomes the shortcomings of local methods, as we show by analyzing the depinning threshold of a single-pin problem.

Keywords: Elasticity; Disorder; Depinning

1. Introduction

Over the past few years relevant progress has been made in the study of disordered elastic interfaces. One of the most intriguing problems concerns the response of the interface to an external force f. Two regimes are observed at zero temperature: (i) When f is smaller than a certain critical threshold f_c, the interface is pinned; (ii) when the force f passes the threshold value ($f > f_c$) the system undergoes the so-called depinning transition [1], which has been widely investigated during the last years [2,3]. The functional renormalization group has allowed to gain a much deeper understanding of this transition [4]. A number of experiments on the contact line of a liquid meniscus on a rough substrate have also been analyzed [5–7].

In this context, we have introduced new algorithms which allow us to solve the depinning problem at zero temperature in finite samples. This paper discusses mathematical aspects of the Variant Monte Carlo (VMC) algorithm, which have not been published yet, although they were implied in past works [8–10]. In Section 2, we prove the no-passing theorem and the forward-moving property for the VMC algorithm, then in Section 3 we discuss in detail the single-pin problem.

The VMC algorithm is able to detect the critical force and the critical configuration (i.e. the ultimate pinned configuration) of a one-dimensional string with

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short-range elasticity moving on a disordered two-dimensional lattice. We have also developed a continuous algorithm [11], which is remarkably useful in higher dimensions and allows to handle long-range interactions.

2. Variant Monte Carlo algorithm

We consider a string $h^t = \{h_i^t\}_{i=0,\dots,L}$ moving at times $t = 0, 1, 2, \dots$ on a spatial square lattice of side L, in a random potential $V(i,h)$ with $h = 0, \dots, M$. The energy of the string is

$$E(h^t) = \sum_{i=1}^{L} \left[V(i, h_i^t) - f h_i^t + E_{\mathrm{el}}\left(|h_{i+1}^t - h_i^t|\right) \right], \quad (1)$$

where f is the external driving force and E_{el} a short-range convex elastic energy. We assume toroidal boundary conditions with a winding term for f such that, at large f, the line keeps winding around the torus, lowering the energy at each time step. In Section 3, we show that a non-local algorithm needs to be used allowing an arbitrary number of points i to move simultaneously by one site in any direction [8].

Following Ref. [8] we define a 'forward front' of length k as a contiguous set of points $i, i+1, \dots, i+k-1$ which move together in forward direction. A 'backward front' is defined similarly. A front is 'unstable' if moving it lowers the energy (1). One has to check only $\sim 2L^2$ fronts to establish whether a string is pinned, i.e. has no unstable front. The 'depinning force' $f_d(h^\alpha)$ of a string h^α is the smallest non-negative f which destabilizes one of its forward fronts. The 'critical force' of a whole sample can then be defined as the largest of the depinning forces of all the strings in the sample

$$f_c = \max_{\{h^\alpha\}} f_d(h^\alpha). \quad (2)$$

The VMC algorithm simply moves a single front of *minimal* length k among the unstable forward and backward fronts. The VMC algorithm is not a valid Monte Carlo algorithm. However, each possible move within the VMC algorithm is also allowed with all the non-local algorithms, and its depinning threshold and ultimate pinned configuration is the same as the one of each non-local algorithm. We will show that the above definition of f_c is appropriate for the VMC algorithm. This implies that it is also correct for general non-local rules, even if they are not restricted to moving fronts only [8].

We stress that these definitions and the following theorems can be easily extended to a general d-dimensional interface with a convex elastic energy. However, the VMC seems to be practically useful only for one-dimensional interfaces with short-range elastic energy as the total number of fronts remains polynomial. We prove the following theorems:

Theorem 1. *Let h^α be a stable configuration. Then the VMC algorithm cannot reach a configuration h^γ with $h_i^\gamma > h_i^\alpha$ for some i from a starting configuration h^β with $h_i^\beta \leqslant h_i^\alpha \forall i$.*

This theorem is illustrated in Fig. 1(a, b, c and d). We suppose the existence of a string h^γ forbidden by the theorem (see Fig. 1(b)):

$$\begin{aligned} &\text{(I)} \quad E(h^\gamma) - E(h^\beta) < 0, \\ &\text{(II)} \quad h_i^\gamma > h_i^\alpha \quad \text{for some } i. \end{aligned} \quad (3)$$

Due to the definition of the VMC dynamics the front connecting h^β to $h^{\gamma'}$ (see Fig. 1(c)) must be stable.

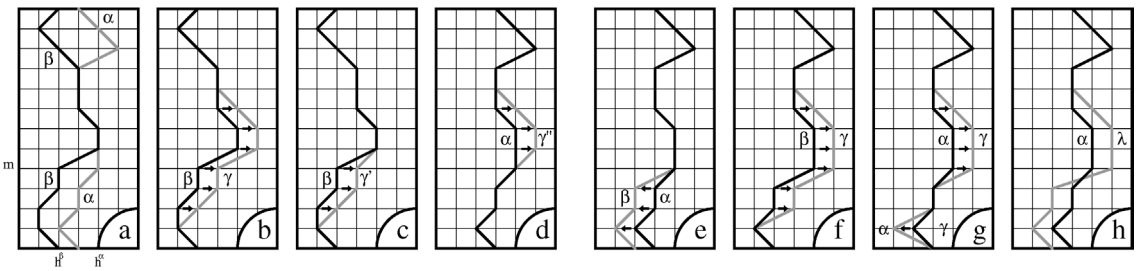

Fig. 1. Illustration of the two theorems.

Moreover, the stability of h^α assures that the front connecting h^α to $h^{\gamma''}$ (see Fig. 1(d)) is also stable:

$$\begin{aligned} &\text{(I)} \quad E(h^{\gamma'}) - E(h^\beta) > 0, \\ &\text{(II)} \quad E(h^{\gamma''}) - E(h^\alpha) > 0. \end{aligned} \tag{4}$$

Subtracting Eq. (3I) from Eqs. (4) and using the expression (1) leads to

$$\begin{aligned} &E_{\rm el}\big(|h_m^\alpha - 1|\big) - E_{\rm el}\big(|h_m^\alpha|\big) + E_{\rm el}\big(|h_m^\beta + 1|\big) \\ &\quad - E_{\rm el}\big(|h_m^\beta|\big) > 0; \end{aligned} \tag{5}$$

where, without any loss of generality, we set $h_{m+1}^\beta = h_{m+1}^\alpha = 0$ (see Fig. 1(a)). From $h_m^\beta < h_m^\alpha$ we write:

$$\begin{aligned} &h_m^\beta \leqslant h_m^\alpha - 1 < h_m^\alpha, \\ &h_m^\beta < h_m^\beta + 1 \leqslant h_m^\alpha. \end{aligned} \tag{6}$$

A convex function $f(x)$ in $[x, y]$ satisfies for all $x_1, x_2 \in [x, y]$:

$$\begin{aligned} &f\big(tx_1 + (1-t)x_2\big) \leqslant tf(x_1) + (1-t)f(x_2), \\ &\quad 0 \leqslant t \leqslant 1. \end{aligned} \tag{7}$$

Taking $x_1 = h_m^\beta$ and $x_2 = h_m^\alpha$, from (6) we can find a t such that:

$$\begin{aligned} h_m^\alpha - 1 &= th_m^\beta + (1-t)h_m^\alpha \\ h_m^\beta + 1 &= th_m^\alpha + (1-t)h_m^\beta. \end{aligned} \tag{8}$$

Using this relation to impose the convexity of the elastic energy in (5) we end up with a contradiction which demonstrates the theorem.

Theorem 2. *Let h^α be pinned in forward direction. Then, the VMC algorithm can at most recede towards a string h^β ($h_i^\beta \leqslant h_i^\alpha \ \forall i$), which is itself pinned in forward direction. The analogous property holds for strings pinned in backward direction.*

An illustration of this theorem is displayed in Fig. 1(e, f, g and h). We suppose that a configuration h^γ, forbidden by the theorem, is reached by the string:

$$\begin{aligned} &\text{(I)} \quad E(h^\gamma) - E(h^\beta) < 0, \\ &\text{(II)} \quad h_i^\gamma > h_i^\alpha \quad \text{for some } i. \end{aligned} \tag{9}$$

The instability of the front connecting h^α to h^β (Fig. 1(e)) implies

$$E(h^\beta) - E(h^\alpha) < 0. \tag{10}$$

We may connect the string h^α to the string h^γ by moving two fronts (see Fig. 1(g)).[1] The forward front is stable because h^α is pinned in forward direction. The backward front is also stable because it is smaller than the front connecting h^α to h^β (VMC dynamics). Thus we conclude:

$$E(h^\gamma) - E(h^\alpha) > 0. \tag{11}$$

Eq. (11) contradicts the sum of (9I) and (10), invalidating the starting hypothesis and proving the theorem.

The 'no-passing theorem' (Theorem 1) assures that the VMC algorithm connects an arbitrary initial state with the critical string, whereas the 'forward-moving theorem' (Theorem 2) allows us to understand that Eq. (2) is indeed appropriate: one might have imagined that the elastic line which cannot advance at f_c could move backwards and then be avoided during the subsequent forward evolution. Theorem 2 excludes the existence of such loopholes. Finally we remark that both theorems transpose correctly to the lattice the analytical properties of the continuum equation of motion [12].

3. Single-pin problem

We now discuss the motion both of a continuous and a discrete elastic line. The line is pinned at a single point which corresponds, with periodic boundary conditions, to $h_0 = h_L = 0$. The equation of motion for the continuous line is

$$\partial h/\partial t = -\partial E_{\rm el}/\partial h + f. \tag{12}$$

A discrete *harmonic* elastic energy $E_{\rm el} = \frac{1}{2}|h_{i+1} - h_i|^2$ then corresponds to the continuous energy $E_{\rm el}(x) = \frac{1}{2}(\partial h/\partial x)^2$, to be integrated over x. The stationary solution under the indicated pinning condition is easily seen to be $h(x) = \frac{1}{2}fx(L-x)$, as shown in Fig. 2 for $L = 10$.

We may also follow the dynamics of the discretized problem from a starting configuration $h_i^{t=0} = 0 \ \forall i$. Of particular interest is the case $f = 1 \pm \epsilon$, with $\epsilon \gtrsim 0$.

[1] In analogy with Theorem 1 we have also to consider the case shown in Fig. 1(h), where we suppose that the line starting from h^β moves to h^λ instead of h^γ. Using the convexity condition (7) the theorem remains valid.

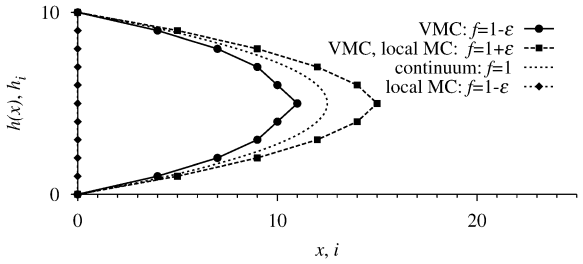

Fig. 2. Single-pin problem with harmonic elasticity. The stationary solution of the VMC algorithm is close to the continuum solution. The stationary solution of the local Monte Carlo algorithm approaches the continuum solution only for $f > f_{\mathrm{loc}} = 1$.

The VMC solutions are given in the figure. They have to be contrasted with the solutions of the local algorithm (only fronts of length 1 can be moved). For $f = 1 - \epsilon$, the starting configuration is stable under local dynamics, as any forward move of a single point costs an elastic energy 1, more than what is recovered through the driving force. The VMC solution is recovered only for $f > f_{\mathrm{loc}}1$. This specific 'critical force' f_{loc} of the local algorithm is independent of L only for the harmonic elastic energy.

The local algorithm is more pathological for stronger than harmonic elastic energies, which have proven to be important in this context [9]. This is evident in the metric constraint model (see [8]). As an example (stronger than harmonic, weaker than metric constraint) we treat a quartic elastic energy $E_{\mathrm{el}} = \frac{1}{12}|h_{i+1} - h_i|^4$ (corresponding to a continuous energy $E_{\mathrm{el}}(x) = \frac{1}{12}(\partial h/\partial x)^4$). The stationary continuum solution of Eq. (12): $h(x) = \frac{3}{8}(\frac{3f}{2})^{1/3}[L^{4/3} - (L - 2x)^{4/3}]$, is again recovered with the VMC algorithm. However, the specific critical force at which the local algorithm becomes equivalent to the VMC method grows with L as $f_{\mathrm{loc}} \sim (\frac{3}{2}f)^{2/3}L^{2/3}$, i.e. diverges with L.

We conclude that the local dynamics is inconsistent even for a single-pin problem. In general disordered samples, it similarly fails to describe the real dynamics of the continuum and is very sensitive to exceptional (local) configurations of the disorder potential, which can block the string even of an infinite systems, and eliminate the interplay between disorder and (collective) elasticity which is at the heart of the depinning problem.

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