Phase separation driven by a fluctuating two-dimensional self-affine potential field

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(February 1, 2008)

We study phase separation in a system of hard-core particles driven by a fluctuating two-dimensional self-affine potential landscape which evolves through Kardar-Parisi-Zhang (KPZ) dynamics. We find that particles tend to cluster together on a length scale which grows in time. The final phase-separated steady state is characterized by an unusual cusp singularity in the scaled correlation function and a broad distribution for the order parameter. Unlike the one-dimensional case studied earlier, the cluster-size distribution is asymmetric between particles and holes, reflecting the broken reflection symmetry of the KPZ dynamics, and has a contribution from an infinite cluster in addition to a power law part. A study of the surface in terms of coarse-grained depth variables helps understand many of these features.

I. INTRODUCTION

The behaviour of a scalar field driven by a fluctuating force field depends strongly on the correlations of the driving field in space and time. A well known example is the passive scalar problem in fluid mechanics, where one asks for the behavior of a passive field as it is advected by a turbulent fluid flow [1]. Even in situations where the driving force field has simpler correlations, the passive scalar field can show interesting, and sometimes unexpected, behaviour. In particular, while in the fluid context an initial local concentration of passive particles typically spreads out in space, in other types of situations an initially randomly distributed set of particles may be driven into a state with large-scale clustering. In this paper, we study one such example.

We consider a force field which is derived from a fluctuating potential, and ask for its effect on a system of particles which do not interact with each other except through hard-core exclusion. The problem is then tantamount to the dynamics of hard-core particles which reside on a fluctuating surface and are driven downwards by gravity along local slopes. An especially interesting case arises when the surface is self-affine with a power-law divergence in the height correlation function as a function of the separation. In such cases, surface roughening strongly affects the clustering of particles and can lead to new types of states [2,3]. We study a stochastically evolving two-dimensional surface governed by Kardar-Parisi-Zhang (KPZ) dynamics [4] and show that surface fluctuations bring about large-scale clustering of particles, akin to phase separation. The particles are taken to be random walkers with an excluded volume constraint, diffusing in the dynamic potential landscape defined by the local height $h(\mathbf{r},t)$ at a base position $\mathbf{r} \equiv (r_x, r_y)$ at time t. In addition, the particles are assumed to be sufficiently massive that the dynamics operates effectively at zero temperature; this means that particles only move locally downwards at a fixed rate, subject to the conditions that the local slope is favourable and the target site is unoccupied. This model is a generalization to two dimensions of the 1-d model studied in [3] where it was found that the particles reach a phase separated state with unusual properties arising from strong surface fluctuations. Since the nature and strength of fluctuations depends strongly on the dimensionality, it is important to see to what extent these features survive in higher dimensions. This is one of the principal aims of this paper.

Let us summarize the main results. Our numerical simulations support the argument that the particle density exhibits phase ordering over a characteristic time-dependent coarsening length scale $\mathcal{L}(t) \sim t^{1/z}$ set by surface fluctuations [3]. Here z is the dynamical exponent for surface fluctuations; for the KPZ surface with $d = 2$, it is known that $z \simeq 1.6$ [5]. The pair-correlation function is found to depend on the separation scaled by $\mathcal{L}(t)$, as is characteristic of a system undergoing phase ordering, but the scaling function has a cusp near the origin, unlike usual phase separating systems [6]. The cluster size distribution in the steady state has a power law decay $N(s) \sim s^{-\tau}$ for $s \ll L^2$, where the exponent τ is different for particles and holes. In addition, unlike the 1-d case, there is a distinct contribution to $N(s)$ from an 'infinite' cluster which contains a finite fraction of the

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total number of particles. An understanding of these results can be gained from a study of the surface itself. To this end, it proves useful to distinguish between regions where the height is less than or more than a fixed reference level. This is incorporated in a Coarse-grained Depth (CD) model of the surface [3,7], which itself exhibits phase separation. Many of its properties reflect the underlying asymmetry of the KPZ surface. Finally, in both the sliding particle and depth models, the order parameter has a distribution that remains broad in the thermodynamic limit.

We introduce the model in Section II. In Section III, we present results for two-point correlation functions, cluster-size distributions and the order-parameter distribution, while Section IV is the conclusion.

II. MODEL

We study an autonomously evolving two-dimensional surface, whose behaviour over large length and time scales is described by the Kardar-Parisi-Zhang equation [4]

$$\frac{\partial h}{\partial t} = \nu \nabla^2 h + \lambda (\nabla h)^2 + \eta(\mathbf{r}, t) \tag{1}$$

with short range correlations for the noise, $\langle \eta(\mathbf{r}, t)\eta(\mathbf{r}', t')\rangle \propto \delta^d(\mathbf{r} - \mathbf{r}')\delta(t - t')$. The KPZ surface in $d = 2$ is known to be self-affine in steady state: $\langle (h(0) - h(\mathbf{r}))^2\rangle \sim r^{2\chi}$ where χ is the roughness exponent. For the KPZ problem with $d = 2$, $\chi \simeq 0.4$ [5,8]. The nonlinear term in Eq.(1) breaks $h \to -h$ symmetry, and this has important consequences for the models we study.

We simulate the surface through a discrete solid-on-solid (SOS) algorithm [9], where the height difference between nearest neighbour (NN) points on a square lattice is maintained at ± 1. A point is selected at random and its height is increased by 2 units with probability p_+ if all four of its NN points are at greater height, and decreased with probability p_- if all four are at a lower height. Otherwise, the site is not updated. It is believed that the asymptotic properties of this single step model are the same as those of the (2+1)-dimensional KPZ equation, though this has not been proved. In our simulations we chose $p_+ = 0$ and $p_- = 1$, so that we have an 'evaporating', rather than a growing surface whose average height decreases in time.

The Sliding Particle (SP) model is defined as follows. Particles are initially distributed at random on surface sites with no more than one particle per site, the overall particle density being ρ. The external force field which drives the particles acts downwards, so that particles tend to move in the same direction as the average surface height, while holes tend to move upwards, opposite to the direction of surface motion. In a microstep, a randomly chosen particle attempts a move to a randomly chosen neighbouring site. If the local slope is favourable and the target site is unoccupied, the move is made, otherwise the particle stays at the same site. One MC step is counted when, on average, all surface sites and all particles have been updated in a random sequence. We verified that a faster rate of updating for particles with respect to surface updates does not change the qualitative results. We did our simulations on square lattices with $\rho = \frac{1}{2}$ and sizes ranging from $L = 32$ to $L = 256$. We used periodic boundary conditions for both the surface and the particles which reside on it.

It is helpful to introduce two sets of discrete Ising-like spin variables to characterise the particle and surface configurations. For the particle configuration, we define $\sigma(\mathbf{r}) = 2n(\mathbf{r}) - 1$ where $n(\mathbf{r})$ is the local occupation index, i.e., $n(\mathbf{r}) = 1$ if there is a particle at $\mathbf{r}$ and zero otherwise. Further, to characterise the height fluctuations of the surface configuration, we define a Coarse-grained Depth model in which we categorize sites according to whether they are above or below a certain fixed height. To this end, we define $s(\mathbf{r}) = -sgn(h(\mathbf{r}) - h_0)$ where h_0 is a chosen reference level. We call the set $\{\sigma(\mathbf{r})\}$ as SP spins and the set $\{s(\mathbf{r})\}$ as CD spins. In order to have a rough correspondence with the half-filled case $\rho = \frac{1}{2}$ of the SP model, we take h_0 to be a spatial average over the configuration of surface heights at that instant.

We expect a correlation between SP and CD spins as local slopes in the surface guide the particles towards the local minima, so that over sufficiently large time scales, particles are expected to preferentially cluster in low-depth regions with predominantly positive CD spins. If particles were to occupy the lowest available positions so as to minimise the total potential energy, we would have a close match of the $\sigma(\mathbf{r})$ and $s(\mathbf{r})$. However, this 'ground state' is never reached as the surface reconfigures itself before particle rearrangements can occur.

III. RESULTS

A. Correlation Functions

The SP-CD correspondence gives an insight into the extent of clustering of the particles. For example, a hill (a region with negative $s(r)$) of linear extension ξ is expected to overturn in typical time $\tau \sim \xi^z$, causing clustering of particles as they fall into the valleys that form. Since the largest hill that overturns within time t has typical size $\mathcal{L}(t) \sim t^{1/z}$, this defines the characteristic length scale for particle clustering [3]. This is verified in a numerical study of the pair spin correlation function $C(r,t) = \langle \sigma(\mathbf{0}, t)\sigma(\mathbf{r}, t)\rangle$ in the SP model. As we see in Fig.1, this function can be fitted into a scaling form $C(r,t) = f(r/\mathcal{L}(t))$ with $\mathcal{L}(t) \sim t^{1/z}$ and $z = 1.6$, which is close to the value of the dynamical exponent for the (2+1) dimensional KPZ surface [5]. This dynamic scaling form is characteristic of a phase ordering system. However, the scaling function has a cusp singularity at small argument, unlike usual coarsening systems where the function is linear for small arguments [6].

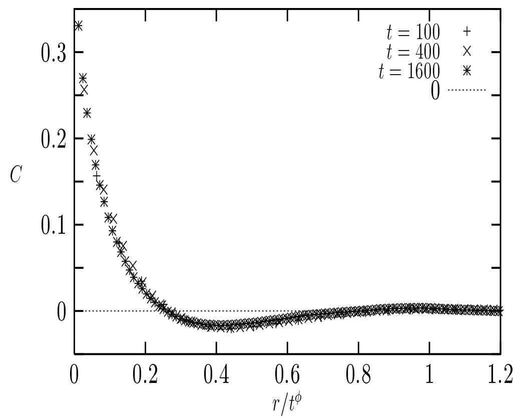

FIG. 1. Equal-time two-point spin correlation for particles sliding down a 2-d KPZ surface of linear size 256. There is a scaling collapse when plotted as a function of the scaled variable r/t^ϕ with $\phi = 0.6$, indicating coarsening. Each point represents an average over 100 different time histories.

In steady state, the system size L replaces $\mathcal{L}(t)$ as the relevant length scale, and a similar scaling form is expected for the correlation function. To quantify the deviation from linearity at small arguments, we studied the structure factor in the steady state,

$$S(\mathbf{k}, L) \equiv \int d^2\mathbf{r} C(\mathbf{r}, L) e^{-i\mathbf{k}.\mathbf{r}}. \tag{2}$$

As shown in Fig. 2, the direction-averaged structure factor is well described by the form $S(k, L) = 1 - c_0 + L^2 g(kL)$, where $c_0 \simeq 0.4$ and $g(q) \sim q^{-(2+\alpha)}$ at large q. The first term arises from a short-distance analytic contribution $(1 - c_0)\delta(\mathbf{r})$ which adds on to the scaling part $f(r/L)$ of $C(\mathbf{r}, L)$. We find $\alpha \simeq 0.38(4)$, a pronounced difference from typical coarsening systems where $\alpha = 1$ (Porod Law) [10]. The non-Porod form implies a cusp in the real space scaling function at small argument,

$$f(x) \simeq c_0 - c_1 x^\alpha + ... \qquad x \ll 1 \tag{3}$$

with $x = r/L$.

We have also studied the two-point correlation function in the CD model, and find a similar behaviour, with a cusp exponent $\alpha \simeq 0.43(3)$ In the next subsection we will show that within the independent interval approximation, the cusp exponent α of the CD model is equal to the roughness exponent χ.

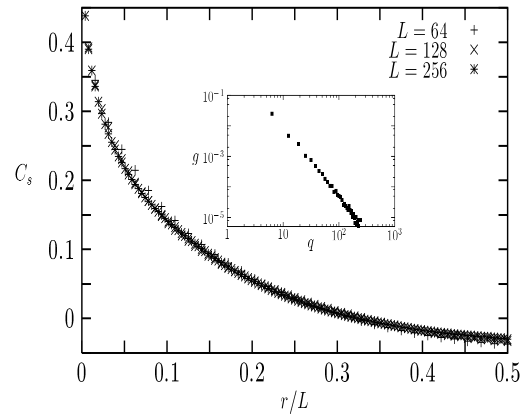

FIG. 2. Steady state pair correlation in the SP model for various system sizes L. The finite size scaling form $C(r, L) = f(r/L)$ illustrated by the data collapse is is characteristic of phase separation. Inset: The scaled structure factor $g(q)$ plotted against the scaled wave vector $q = kL$ with $L = 128$ shows that $g(q) \sim q^{-(2+\alpha)}$ with $\alpha \simeq 0.38(4)$, implying a cusp singularity in the real space correlation function.

B. Cluster Size Distributions

Let us define a cluster as a set of like SP spins (particles or holes), each of which is a nearest neighbor of at least one other like spin in that cluster. A study of the size distribution of clusters shows (Fig. 3) that the number of connected clusters $N_\pm(s)$ with s particles (holes) has a power-law decay for $s \ll L^2$:

$$N_\pm(s) \sim L^2 s^{-\tau_\pm} \quad ; \quad s \ll L^2 \tag{4}$$

where $\tau_+ \simeq 2.2$ and $\tau_- \simeq 2.0$. This power-law distribution of cluster sizes, reminiscent of critical systems, is another characteristic feature of the unusual phase separated state under study — it occurs in one dimension as well [3]. There are, however, two important differences from the 1-d case. First, there is a marked difference in the powers τ_+ and τ_- for particle ($\sigma_i = +1$) and hole ($\sigma_i = -1$) clusters, which reflects the asymmetry of the $s_i = +1$ and $s_i = -1$ clusters in the CD model as discussed below. Second, for the particle cluster distribution we find that there is an additional large s contribution of the form $f_\infty(s/L^2 - y_0)$ peaked at $y_0 \simeq 0.4$. For finite system sizes, f_∞ is somewhat broad, but with increasing L, the width of the peak narrows down. We find that the area under the peak is unity, implying that there is a single very large cluster in every configuration. Also, the fraction of particles contained in this cluster is $2y_0 \simeq 0.8$.

The power-law distribution of cluster sizes in the SP model has its counterpart in the CD model too. It is known that when a rough surface is intersected by a horizontal plane, the distribution of areas enclosed by the closed contours of intersection has the power-law form $\mathcal{N}(s) \sim s^{-\tau^*}$ for $s \ll L^2$, where $\tau^* = 2 - \frac{\chi}{2}$ [11–13]. A typical contour encloses several other contours, and the overall structure is scale invariant [9]. For the KPZ surface one should moreover distinguish between contours whose inner perimeter sites lie above or below the cut, as there is no *a priori* reason for both the distributions to be identical. In fact, numerical simulations show that cluster size distributions for CD spins (which are closely related to area distributions), indeed has an asymmetry between positive and negative spins (Fig. 4). Both the distributions follow power-law decays, but with different exponents. The exponent for negative CD spins is numerically close to τ^*, while that for positive spins is significantly larger. Morover, there is a contribution from an infinite cluster of positive spins, as for the particle distribution in the SP problem.

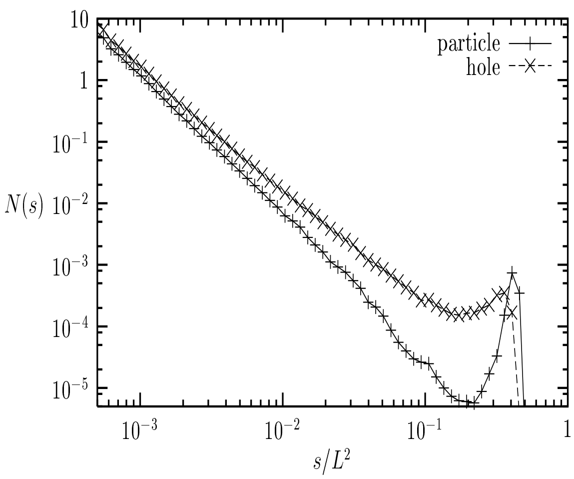

FIG. 3. Size distribution of cluster sizes for + spins (particles) and − spins (holes) for the SP model. The data shows a power-law decay with exponent $\simeq 2.2$ and a well-separated 'infinite' cluster for particles, and a lower value of the exponent $\simeq 2.0$ for holes. We used $L = 128$ and averaged over 100 histories.

Within the CD model, we argue that power laws in cluster distributions of a different sort are related to the occurrence of a cusp in the scaled correlation function. For a self-affine surface with roughness exponent χ, it is known that the probability $P(l)$ that the surface first returns to its starting height $h(\mathbf{x} = \mathbf{0}) = h_0$ after moving a distance l along an arbitrary linear direction has a power-law decay at small l: $P(l) \sim l^{-(2-\chi)}$ for $l \ll L$ [7,11,14]. Each such segment defines a linear cluster of CD spins s_i of the same sign, along the linear cut. Now let us make the independent interval approximation (IIA) in which the lengths of such segments are taken to be independent random variables. This enables the Laplace transforms of the cluster size distribution and pair correlation function for CD spins (defined relative to h_0) to be related along any linear cut. The nonstandard feature is that the mean cluster size diverges as $L \to \infty$, but the correlation function can be calculated as in [3]. It has the scaling form

$$C^*(r, L) \simeq 1 - a(\frac{r}{L})^\chi + .. \quad ; \quad r \ll L \quad (IIA) \qquad (5)$$

Comparing with Eq.3, we see that the IIA predicts that the cusp exponent α in the CD model is equal to the roughness exponent χ. The KPZ value χ is quite close to the measured value of α for the CD model, and also to that for the SP model. The behaviours of both models on large scales of distance and time appear to be similar in 2-d, even though the microscopic configurations of the two match only roughly. To get an idea of the latter, we monitored the overlap index $O = \langle \sigma(\mathbf{r}) s(\mathbf{r}) \rangle$, and found that O varies between $\simeq 0.38$ when the frequency of updates of particles and surface is equal, and a saturation value $\simeq 0.6$ as the ratio between the two is increased. However, there was no corresponding significant change in the numerical values of the exponents α and τ.

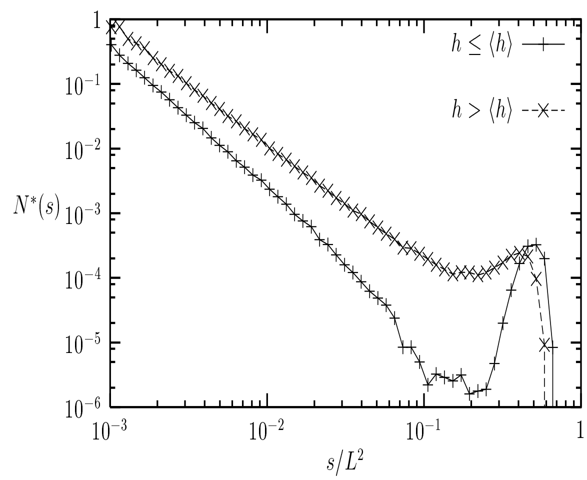

FIG. 4. Domain size distribution for + (valley) and −(hill) spins for the CD model. The exponents for the power-law parts have values $\simeq 2.2$ and 1.85 respectively. There is a distinct contribution to the distribution of + spins from an infinite cluster. We used $L = 128$ and averaged over 100 histories.

C. Order Parameter

For a system with conserved magnetisation like the SP model, an appropriate quantity to characterise the ordered state is the steady state average of the magnitude of the Fourier components of the density [3], defined as $Q(\mathbf{k}) = \langle |L^{-2} \sum_{\mathbf{r}} n(\mathbf{r}) e^{-i\mathbf{k}.\mathbf{r}}| \rangle$ where $\mathbf{k} = \frac{2\pi}{L}(n_x, n_y)$ and $|\mathbf{k}| \leq \pi$. Taking the magnitude guarantees that $Q(\mathbf{k})$ receives the same contribution from all configurations that can be obtained from each other by translational shifts [15]. In Fig. 5, we plot $Q(\mathbf{k})$ along the (1,0) direction for four different lattice sizes. The sequence of curves suggests that for any fixed, finite k, $Q(k = 2\pi n/L, 0)$ approaches zero as L increases. However, if n is held fixed so that $|\mathbf{k}|$ approaches zero as $L \to \infty$, the corresponding Q approaches a finite limit. Of this set of Q's, the largest is $Q^* = Q(\frac{2\pi}{L}, 0)$, and provides the simplest characterization of the order.

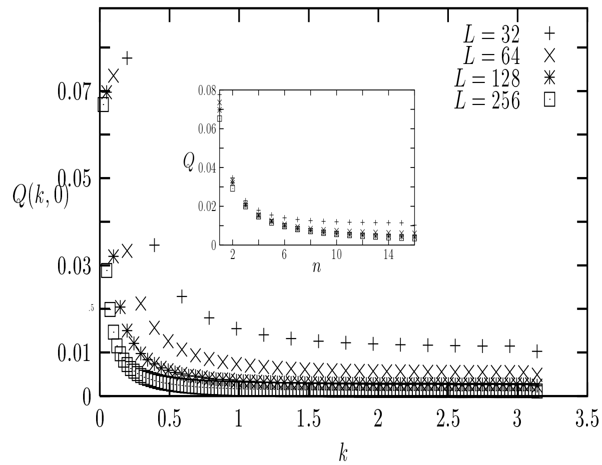

FIG. 5. $Q(k, 0)$ plotted against wave vector $k = 2\pi n/L$ and (Inset)n for four lattice sizes.

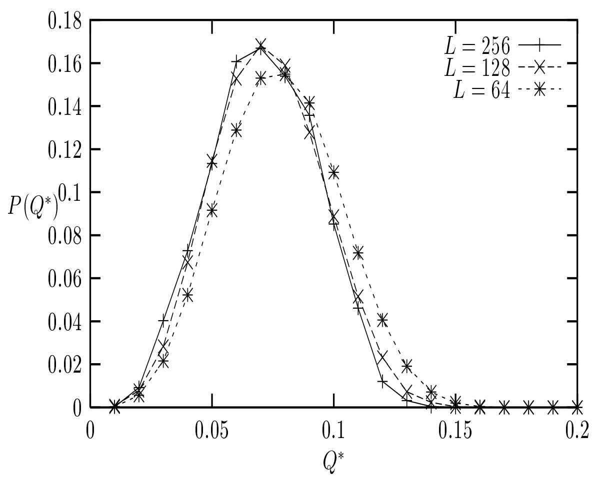

FIG. 6. Probability distribution of the order parameter Q^* for three lattice sizes for the SP problem.

Fluctuations in the SP model are unusually strong and are reflected in the probability distribution of Q^* (Fig. 6). The distribution seems to remain broad and approach a limit as L increases, with $\langle Q^* \rangle \simeq 0.07$ and variance $\simeq 0.02$. Similar studies of the corresponding CD model shows that there is a broad distribution there as well, and we find $\langle Q^* \rangle \simeq 0.11$. The fact that the RMS fluctuation of the order parameter does not vanish in the large-size limit is an unusual and characteristic feature of the ordered state of this model. Note that fluctuations which drive Q^* towards zero need not take the system into a disordered state. A study of the temporal fluctuations of Q^* in one dimension showed that a low value of Q^* occurs simultaneosly with an increase of the value of Q for another close-by n, so that the state retains macroscopic order, but with a few more coexisting macroscopic domains [3]. A more complete characterization of the order in two dimensions would thus involve finding the joint probability $\mathcal{P}[Q(\frac{2\pi n_x}{L}, \frac{2\pi n_y}{L})]$ as $L \to \infty$, but this has not been attempted here.

It is interesting to compare the distribution $P(Q^*)$ for this model with the corresponding quantity for a more familiar system such as the 2-d Ising model evolving under conserved (Kawasaki) dynamics. For the ferromagnetic Ising model with equal numbers of up and down spins, the ordered state in a finite system consists of strips of width $\sim \frac{1}{2}L$ parallel to either x or y axes, with equal probability. Thus the distribution $P(Q^*)$ (say, with $Q^* = Q(\frac{2\pi}{L}, 0)$) in that case would have two peaks, one at a non-zero value of Q^* corresponding to strips forming along the x-direction, and another peak at $Q^* = 0$ which corresponds to strips forming in the y-direction. In our case, however, the peak at the origin is absent as the interface between phases is much more diffuse and there is no strip formation. In this sense, the ordering observed in this model is very different from that in traditional equilibrium models.

IV. CONCLUSION

To conclude, we have studied a model where a fluctuating self-affine surface drives a set of downward-drifting particles to a phase separated state. The phase separation has several unusual characteristics arising from the presence of strong fluctuations which survive even in the thermodynamic limit. These include a power-law distribution of cluster sizes, a cusp in the scaled pair correlation function and a finite width of the order parameter distribution. These features mirror the properties of a coarse-grained height model of surface fluctuations, where they follow directly from the self-affine nature of surface fluctuations. In particular, the asymmetry in the cluster size distribution for particles and holes is a consequence of the fact that KPZ growth breaks up-down symmetry. It would be interesting to see if a similar asymmetry exists in other related quantities such as the distribution of lengths of contours and the areas enclosed by them.

It would also be interesting to study the sliding particle problem on a fluctuating Edwards-Wilkinson surface, where particle-hole symmetry should be restored in the half-filled case. This surface is logarithmically rough in 2-d, suggesting that the scaled two-point correlation functions for the sliding particle and depth problems should show an even sharper cusp than for the KPZ surface studied in this paper.

Finally, we remark that it would be interesting to explore the effects of removing the hard core interaction between particles. A study of noninteracting particles sliding on a KPZ surface in one dimension indicates a power law decay of the two-point correlation function [2]. A study of other characteristics of the resulting state should prove quite revealing.

V. ACKNOWLEDGEMENTS

We would like to thank D. Das, D. Dhar, S.N. Majumdar, B. Schmittmann and R.K.P Zia for helpful discussions. G. M. acknowledges the hospitality of the Tata Institute of Fundamental Research where this work was initiated. This research is supported in part by a grant (DMR-0088451) from the US National Science Foundation.

It is a pleasure and a privilege to contribute this article to the Festschrift volume for the 70th birthday of Prof. Michael E. Fisher, whose work on various aspects of co-operative ordering has inspired several generations of statistical physicists. MB would like to acknowledge many stimulating interactions over the years with Professor Fisher, both professional and personal.

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