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Surface growth and crossover behaviour in a restricted solid-on-solid model

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Abstract. We describe results of numerical simulations of growth in a restricted solid-on-solid model. We first extract the exponent β by comparing the surface width $W(t) \sim t^{\beta}$ with a spatially averaged height correlation function $\overline{G}(t)$. The latter is shown to give a more accurate estimate for β, even for relatively small systems. The exponent χ is obtained from the saturation of the interface fluctuations in the late time regime. Our results lead to a conjecture of dimension dependent exponents as $\beta(d) = 1/(d+1)$, $\chi(d) = 2/(d+2)$. In addition, we study time dependent crossover phenomena by relaxing the local height constraint, and using a noise reduction method in the model. We demonstrate how the effect of such crossover effects may lead to spurious values of the growth exponents. Finally, we discuss our results in relation to other discrete models, and the continuum growth equations.

1. Introduction

Over recent years, there have been considerable efforts in studying various models of externally driven growth of clusters and surfaces far from equilibrium (Krug and Spohn 1990b). In the simplest possible non-trivial case, such processes may be completely determined by the effect of random deposition and subsequent local surface diffusion (Edwards and Wilkinson 1982). However, in more realistic models the interactions between particles on the surface must be taken into account, leading to the presence of more complicated nonlinear processes which determine the fluctuations of the growing interface (Kardar *et al* 1986) in the Eden model (Eden 1961) or ballistic deposition model (Family and Vicsek 1985, Meakin *et al* 1986). These processes are also related through various mappings to other physical problems such as the Burgers' equation (Burgers 1974) in fluid mechanics, or the thermodynamics of directed polymers in random media (Kardar and Zhang 1987). The nonlinear processes controlling these systems are still not completely understood despite their superficially simple mathematical representation. In particular, higher dimensional values for the scaling exponents in the strong coupling regime of the nonlinearities are still under dispute, as we will elucidate in the following.

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In considering the problem of a driven surface, it is natural to characterize the surface by the width $W(L,t)$ which is defined as the standard deviation of heights, i.e.

$$W^2(L,t) = \frac{1}{L^{d_s}} \int d\boldsymbol{r}\, [h(\boldsymbol{r},t) - \bar{h}(t)]^2 \tag{1.1}$$

where $h(\boldsymbol{r},t)$ are the local height variables of the $d_s = (d-1)$-dimensional interface, $\bar{h}(t)$ is their spatial average, and L is the linear size of the substrate. Based on computer simulations of growth in various discrete models, it has been found that $W(L,t)$ obeys the scaling relation (Family and Vicsek 1985)

$$W(L,t) \sim L^{\chi} f(\frac{t}{L^z}) \tag{1.2}$$

where the scaling function $f(x)$ is proportional to x^{β} for $x \ll 1$, with $\beta \equiv \chi/z$ and becomes constant for $x \gg 1$. The surface width has been commonly used in simulations to obtain estimates for the growth exponents β and χ. However, the most complete current description of a growing interface in the continuum limit has been given by Kardar, Parisi and Zhang (KPZ), (1986). The KPZ equation explicitly takes into account the relevant nonlinearities associated with surface growth as

$$\frac{\partial h}{\partial t} = \nu \nabla^2 h + \lambda (\nabla h)^2 + \eta(\boldsymbol{r},t) + \mu \tag{1.3}$$

where μ is a constant driving force and η is a Gaussian random variable which satisfies

$$\langle \eta(\bar{r},t)\eta(\bar{r}',t') \rangle = 2D\delta(\bar{r}-\bar{r}')\delta(t-t') \tag{1.4}$$

with D describing local variations in the deposition rate. In the trivial case $\nu = \lambda \equiv 0$, the KPZ equation describes a simple uncorrelated random deposition model, for which the only relevant exponent $\beta = 1/2$. In the case of an ideal interface, for which $\lambda \equiv 0$, equation (1.3) can be solved exactly for the height–height correlation function

$$\lim_{t_0 \to \infty} \langle (\hat{h}(\boldsymbol{r}, t+t_0) - \hat{h}(0,t_0))^2 \rangle \sim r^{2\chi} \bar{f}(rt^{-1/z}) \tag{1.5}$$

with $\hat{h}(\boldsymbol{r},t) = h(\boldsymbol{r},t) - \bar{h}(t)$, leading to scaling exponents $\beta = (3-d)/4$ and $\chi = (3-d)/2$ below an upper critical dimension $d_c = 3$ (Edwards and Wilkinson 1982). Above d_c, the interface is smooth and logarithmically rough at d_c with $\beta = 0$, while $z = 2$ independent of d. Finally, in the most general case when both $\lambda \neq 0$ and $\nu \neq 0$, the KPZ equation has only been solved in $d = 2$, where $\beta = 1/3$ and $\chi = 1/2$ (Forster *et al* 1977, Huse *et al* 1985, Kardar *et al* 1986). An invariance of the equation under infinitesimal tilt of the interface also yields a relation $\chi + z = 2$ between the scaling exponents (Medina *et al* 1989). For $d \geqslant 3$, there have been considerable efforts to pin down the scaling exponents. Renormalization group analysis of the KPZ equation reveals that the strength of the nonlinearity is controlled by the coupling constant $g \equiv \lambda^2 D/\nu^3$ (Forster *et al* 1977, Kardar *et al* 1986). For g sufficiently small, the interface is ideal with $\beta = 0$ and $z = 2$. However, in the physically interesting strong coupling regime, analytic theories (McKane and Moore 1988, Halpin-Healy 1989a, Cook and Derrida 1990) and numerical simulations (Meakin *et al* 1986, Zabolitzky

and Stauffer 1986, Wolf and Kertész 1987, Kim and Kosterlitz 1989a, Forrest and Tang 1990) on various growth models yield results which currently disagree with each other. Furthermore, recent simulations in some discrete growth models have suggested the possibility of dynamical 'phase transitions', leading to possible different exponents (Yan *et al* 1990, Guo *et al* 1990, Pellegrini and Jullien 1990).

In this work, we have undertaken a detailed analysis of numerical simulations in the restricted solid-on-solid (RSOS) growth model (Kim and Kosterlitz 1989a). We demonstrate that minimization of the RSOS height constraint leads to the appearance of a well defined scaling regime for the model, which can be used to estimate accurate values for the growth exponents. By comparing various definitions for the surface width, we show that the spatially averaged height correlation function $\overline{G}(t)$ yields the most accurate and reliable estimates for β, even for relatively small system sizes. In the $d = 1 + 1$ dimension, our results reproduce the exact results for the KPZ equation. In $d = 2+1$, we obtain from our best data the results $\beta = 0.250 \pm 0.005$ and $\chi = 0.40 \pm 0.01$. Taking the relation $\chi + z = 2$ (Meakin *et al* 1986, Krug 1987, Medina *et al* 1989) to be exact, these results together with our somewhat less accurate estimates up to $d = 4 + 1$ for β, lead to the conjecture of dimension-dependent exponents as (Kim and Kosterlitz 1989a)

$$\beta(d) = \frac{1}{d+1}$$
$$\chi(d) = \frac{2}{d+2} \tag{1.6}$$
$$z(d) = \frac{2(d+1)}{d+2}.$$

This conjecture, although not in agreement with some other simulation results (Meakin *et al* 1986, Wolf and Kertész 1987, Forrest and Tang 1990), nevertheless reproduces exactly the known limits in $d = 1 + 1$, and implies that there is no finite upper critical dimension (Wolf and Kertész 1987, Halpin-Healy 1989b). In order to understand the origin of these seemingly different results obtained from simulations of other discrete growth models, we relax the height constraint and introduce noise reduction into the RSOS growth model. This leads to the appearance of strong crossover effects making a quantitative determination of the growth exponents difficult. We examine the nature of these crossover effects in detail, and discuss our results in relation to the other discrete models, and to the continuum KPZ equation.

2. RSOS growth model

The class of models known as solid-on-solid (SOS) models have been extensively studied as simple models of the equilibrium properties of surfaces, in particular surface steps. The existence of a Kosterlitz–Thouless (1973) roughening transition (RT) on surfaces, for example, was first realized in the three-dimensional SOS model (Weeks 1980). The characteristic feature of all models within this class is the restriction of fluctuations to exclude all configurations with overhangs, bubbles and lattice vacancies. An important variation among the SOS models is the RSOS model, in which the differences between neighbouring heights of the local columns $|\Delta h|$ are usually restricted to zero or unity

in magnitude. Even with this restriction, the RSOS model still exhibits a RT at three dimensions.

SOS models have also been studied in the context of non-equilibrium phenomena, such as surface growth (Kim and Kosterlitz 1989a, Amar and Family 1990a, Guo *et al* 1990). However, no conclusive studies have so far been made in order to understand the fundamental non-equilibrium properties, or the nature of growth processes in these models as we have discussed in the introduction. To address these questions, in this work we consider a particularly simple aggregation model, which we call the restricted solid-on-solid growth (GRSOS) model. As described later, we shall present results of comprehensive studies of computer simulations for externally driven surface growth in this model.

We define the RSOS surface growth model as a ballistic growth model driven by external uncorrelated noise. Particles of height unity are randomly deposited on a $d_s = (d-1)$-dimensional substrate of columns of heights $\{h_i(t=0)\} = \{0\}$, which is initially flat without any thermal fluctuations. The ballistically deposited particles are incorporated into the substrate *if and only if* the height difference between all nearest-neighbour columns satisfies the local RSOS condition $|\Delta h| \leqslant N$, where N is a fixed, positive integer. If this condition is not met, the corresponding particle is rejected from the system.

Within this formulation, the crucial parameter in the model is the adjacent column height difference restriction N. In the limit where $N \to \infty$, the GRSOS model becomes identical to the random deposition model, for which the growth exponent $\beta = 1/2$ in all dimensions. However, in the opposite limit where N is small, the local restrictions on column heights play an important role. In fact, as we shall show later, minimizing the height restriction seems to greatly reduce short-wavelength fluctuations and suppress lateral growth compared to other ballistic growth models and the Eden (1961) model, and thus facilitates reaching the asymptotic growth regime of the model. In fact, simple arguments based on the growth of steps reveal that, for the GRSOS model, λ is negative with a large absolute value while, for the Eden model and other similar ballistic growth models, $\lambda > 0$ (Kim 1989). However, since the sign of λ is irrelevant, we expect these models to belong to the same universality class.

2.1. Simulations of growth exponents

We have carried out standard Monte Carlo simulations for the GRSOS model for various dimensions and values of N, in order to determine the relevant exponents governing the growth process. Most simulations were done for the minimum value of $N = 1$ with fully periodic boundary conditions, starting from an initially flat substrate. We shall also discuss later the effect of systematically relaxing the height constraint N. Time in the simulations is measured in units of the average height $\bar{h}(t) \equiv \langle h_i(t) \rangle$, where $\langle\ \rangle$ denotes averaging over space. We note that a somewhat natural definition of time t_{MC} is the number of Monte Carlo steps. These differ by small finite size effects $\bar{h}(t_{MC}) \sim t + at^{\beta}$ where the amplitude a is very small for the RSOS model (Krug and Meakin 1990).

We have monitored the growth process by calculating the width W of the surface using two different definitions. The surface width W_a on the active sites is defined by

$$W_a^2 = \frac{1}{N_a} \sum_{i=\text{active}} (h_i - \bar{h})^2 \tag{2.1}$$

where h_i is the height of columns in the active zone, and N_a is the total number of columns in the active zone in which particles can be added without breaking the local height restriction. Another measure of the surface width is defined on the whole region of the substrate by

$$W^2 = \frac{1}{N_0}\sum_i (h_i - \bar{h})^2 \tag{2.2}$$

where the sum now goes over all column heights of the substrate with a total mean height $\bar{h}$, and $N_0 = L^{d_s}$ is the total number of columns. The scaling properties of $W(t)$ and $W_a(t)$ are equal in the limit of very large systems, but our systematic comparisons between the two definitions of the width discussed in section 2.1.2 reveal that W in equation (2.2) turns out to give better estimates of exponents for systems of given size L.

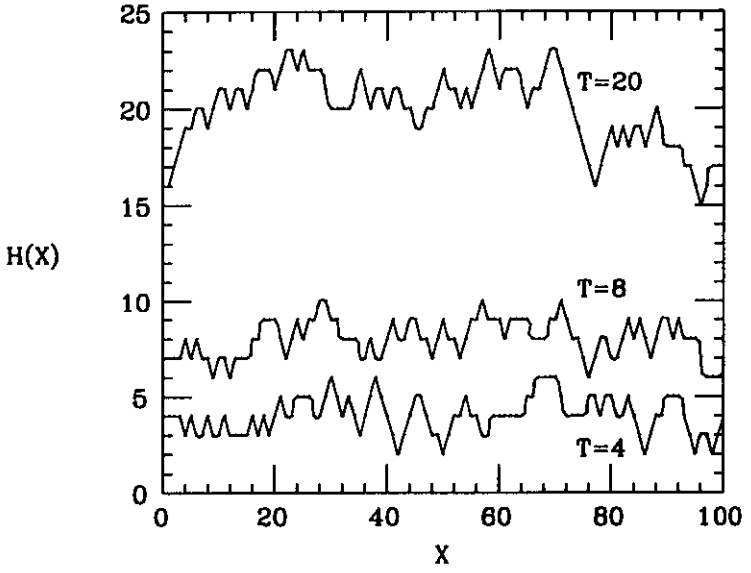

Figure 1. Temporal development of fluctuations of the interface $\{h_i(t)\}$ in $d = 1+1$ GRSOS model for $t = 4, 8, 20$. The interface is initially flat at $t = 0$.

In figure 1 we show an example of the topology of the growing surface for $N = 1$, $d = 1 + 1$ and $L = 100$. Starting from a flat surface, the fluctuations of the surface width increase with time and become saturated when the parallel correlation length becomes proportional to the size of the system. Depending on the extent of these fluctuations, we can divide the growth process in approximately three different regimes.

(i) For very early times $t \ll 1$ when the density of deposited particles is low, the height restriction plays virtually no role in the deposition process. We then expect $W(t)$ to be proportional to the random deposition result $t^{1/2}$. This transient regime results from the flat initial surface used in the simulations.

(ii) For $1 \ll t \ll L^z$ we expect the system to be in the scaling region of the growth, in which a power law behaviour $W(t) \sim t^{\beta}$ should be observed, as the parallel

correlation length grows as $\xi_{\|}(t) \sim t^{1/z}$. In this regime the height restriction plays a crucial role in determining the temporal development of the fluctuations and the exponents.

(iii) For very late times $t \gg L^z$ the parallel correlation length of the surface has saturated and span the size of the system with $\xi_{\|} \sim L$. In this regime the behaviour of the surface width is controlled by the roughness exponent χ, such that $W(L) \sim L^{\chi}$. However, we still expect the height restriction to play an important role in determining the value of χ.

In order to reliably obtain the scaling exponents β and χ, we will describe the behaviour of the interface in the GRSOS model separately for the regimes (ii) and (iii).

2.1.1. Rate of interface growth. To determine β, the exponent governing the rate of growth of the interface width, we have first used the relation of $W(t) \sim t^{\beta}$. In figure 2 we display on a logarithmic scale the time dependence of $W(t)$ for systems of the sizes $L = 6144$ $(d = 1+1)$, 512 $(d = 2+1)$, 64 $(d = 3+1)$, and 46 $(d = 4+1)$. In each case, the minimum value $N = 1$ was used for the height restriction parameter. A careful analysis of the very early time regime reveals a random deposition exponent $\beta = 1/2$ in all dimensions, which crosses over to another, non-trivial value typically already after $t \geqslant 4$. Using standard least-squares linear fitting to our data, we can summarize our results as follows

$$\beta = \begin{cases} 0.332 \pm .005 & d = 1+1 \\ 0.248 \pm .005 & d = 2+1 \\ 0.195 \pm .01 & d = 3+1 \\ 0.155 \pm 0.02 \sim 1/6 & d = 4+1. \end{cases} \tag{2.3}$$

The time ranges used in each case are $4 \leqslant t \leqslant 640$ for $d = 1+1$, $4 \leqslant t \leqslant 64$ for $d = 2+1$, $4 \leqslant t \leqslant 12$ for $d = 3+1$, and $4 \leqslant t \leqslant 8$ for $d = 4+1$. In each case, several additional system sizes were used to compute β. These results are our best estimates of the true size independent exponents, and the result in $d = 1+1$ agrees well with the exactly known answer $\beta = 1/3$. However, we must note that for the last case of $d = 4+1$, the surface width is initially clearly oscillating (see figure 2), as the surface width is small compared to unity, and the substrate size is relatively small. Thus, the corresponding estimate for β is not very accurate. Finally, we have also calculated $W(t)$ for a 128×128 triangular substrate in $d = 2+1$ with $N = 1$, and estimate $\beta = 0.247 \pm .01$, for $4 < t < 32$. As expected, this is consistent with the assumption that the growth exponents within the model are universal and independent of the underlying lattice structure.

2.1.2. Saturation of interface fluctuations. The roughness exponent χ describes the saturation of the interfacial fluctuations in the late time regime. As we have discussed previously, this occurs when the parallel 'correlation length' $\xi_{\|}$ associated with the surface becomes comparable to the system size L. In this late time regime we can then determine χ from the relation $W(L) \sim L^{\chi}$. The system in this regime has become 'self-critical' in the same sense as many other dynamical systems, which start at rest and finally display power law behaviour of fluctuations in a late time steady state regime (Bak *et al* 1987). Since the surface width is calculated from a fluctuation relation (Milchev *et al* 1986), we expect W to display lack of self-averaging in the

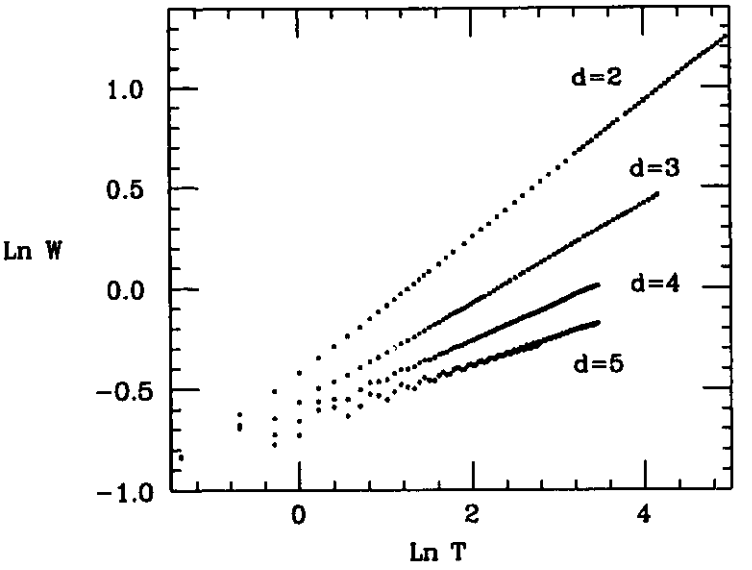

Figure 2. Interface width $W(t)$ against time on a logarithmic scale for various dimensions. The slope of each curve gives the growth exponent β, as discussed in the text.

sense that the relative fluctuation (the run-to-run fluctuation of W divided by the average of W) remains constant as the system size increases in the regime (iii). This has been verified numerically (Kim 1989). Note that, in the saturated regime where fluctuations are limited by system size, averaging over time and runs are equivalent.

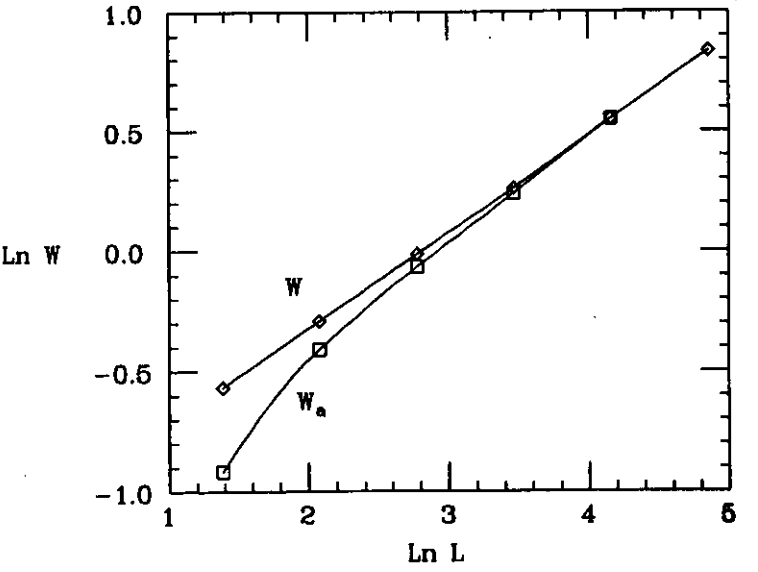

Figure 3. Comparison between the two definitions (2.1) and (2.2) for the interface width in $d = 2 + 1$, plotted against system size in the saturated regime (iii). The width defined over the whole surface in equation (2.2) gives better scaling behaviour for smaller systems.

Before computing χ from the saturation of the interface width, we performed systematic comparisons between the two possible definitions of W. In figure 3 we display a comparison between (2.1) and (2.2) as a function of system size L for $d = 2+1$, in the saturated regime. As we can clearly see from the data, W as defined over the whole surface, shows better scaling behaviour for small system sizes. In the limit of very large L, both definitions of the width agree, as expected. However, to reliably determine χ we have used the definition (2.2) in our calculations.

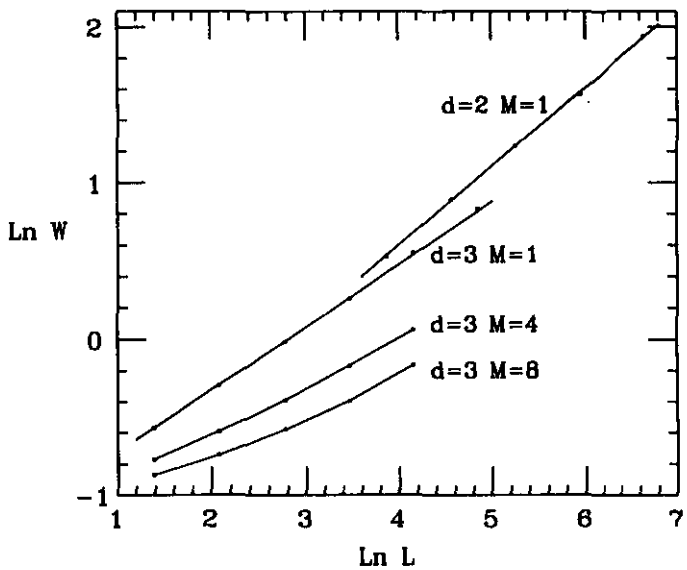

Figure 4. Interface width in the saturated regime $W(L) \sim L^{\chi}$. The effect of the noise reduction parameter M is also shown (cf section 2.2.2).

Our simulations were restricted to relatively small systems $L \leqslant 768$ for $d = 1 + 1$ and $L \leqslant 128$ for $d = 2 + 1$. The time required to reach the saturated regime is larger than about $L^{1.5}$ in $d = 1 + 1$ and $L^{1.6}$ in $d = 2 + 1$. In each case, the surface width was averaged over 2000 independent runs. In figure 4 we depict the results for $W(L)$ in two and three dimensions on a logarithmic scale. Using again a straight line fit to the two curves we obtain the following results :

$$\chi = \begin{cases} 0.50 \pm 0.01 & d = 1+1 \quad N = 1 \\ 0.40 \pm 0.01 & d = 2+1 \quad N = 1. \end{cases} \tag{2.4}$$

The result in $d = 2$ produces the exact answer $\chi = 1/2$ rather accurately. As expected, combining these numbers with our results for β, the scaling relation $z+\chi = \chi/\beta+\chi = 2$ is satisfied to better than 1% within our numerical accuracy.

2.1.3. The height correlation function. There exists another important quantity, which we can use to independently determine the growth exponent β. This is the height difference correlation function

$$G(\boldsymbol{r}, t) \equiv \langle [h(\boldsymbol{x} + \boldsymbol{r}, t) - h(\boldsymbol{x}, t)]^2 \rangle_{\boldsymbol{x}} \tag{2.5}$$

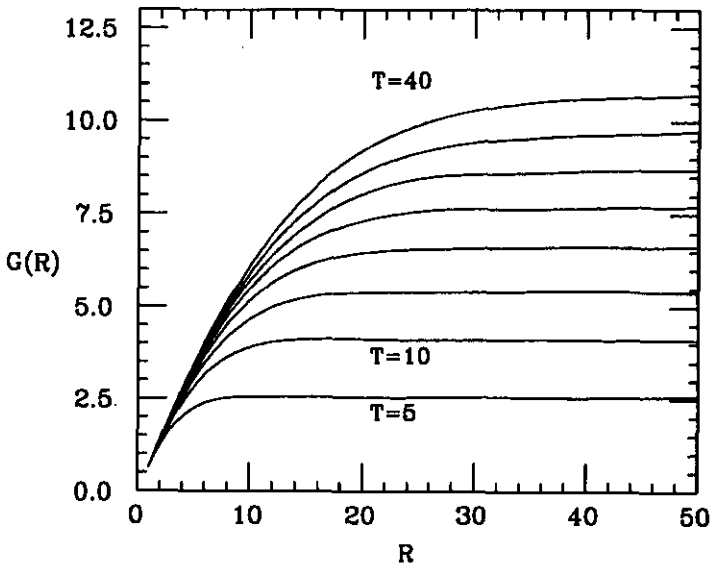

Figure 5. Height correlation function $G(\boldsymbol{r},t)$ plotted at fixed times $t = 5, 10, \ldots, 40$ against distance r in $d = 1 + 1$. The saturated values can be used to obtain an accurate estimate of β.

where $\langle\ \rangle_{\boldsymbol{r}}$ denotes an average over all lattice positions and configurations. Since $G(\boldsymbol{r},t)$ is periodic and $G(\boldsymbol{r},t) = G(-\boldsymbol{r},t)$, we can compute $G(\boldsymbol{r},t)$ on the range $0 \leqslant r \leqslant L/2$. From the scaling relations for the correlation function:

$$\begin{aligned} G(\boldsymbol{r},t) &\sim L^{2\chi} f(r/L) \\ &\sim r^{2\chi} \qquad \text{for } r \ll L \\ &\sim L^{2\chi} \qquad \text{for } r \approx L/2 \end{aligned} \tag{2.6}$$

for $t \gg L^z$, and

$$\begin{aligned} G(\boldsymbol{r},t) &\sim t^{2\beta} \hat{f}(r/t^{1/z}) \\ &\sim r^{2\chi} \qquad \text{for } r \ll t^{1/z} \\ &\sim t^{2\beta} \qquad \text{for } r \gg t^{1/z} \end{aligned} \tag{2.7}$$

for $t \ll L^z$, we can see that at a fixed, early time $t \ll L^z$, $G(\boldsymbol{r},t)$ becomes constant for $\xi_{\parallel}(t) \sim t^{1/z} < r$. In figure 5 we show results of numerical calculations of the correlation function for $t = 5, 10, 15, \ldots, 40$ as a function of r, for $L = 512$ in $d = 1 + 1$. The asymptotic constant value of the flat region of G can be used to compute the exponent β by defining an average quantity $\overline{G}(t)$ as

$$\overline{G}(t) \equiv \langle G(\boldsymbol{r},t) \rangle_{r} \tag{2.8}$$

where the spatial average $\langle\ \rangle_{r}$ was computed in the range $L/4 < r < L/2$ at fixed $t \ll L^z$ to reduce fluctuations. For $d = 2 + 1$, the spatial average of $G(\boldsymbol{r},t)$ was done in four separate directions only to reduce the computing time required.

As we can see from the scaling relations (2.6) and (2.7), the average value $\overline{G}(t) \sim t^{2\beta}$. Using our data from figure 5, and plotting $\ln[\overline{G}(t)]$ against $\ln(t)$, we obtain $\beta = 0.334 \pm 0.005$ in $d = 1 + 1$, which is again very close to the exact value 1/3. To study the finite size effects we did a comprehensive analysis of data for a $L = 256$ system in $d = 2 + 1$, averaged over 100 configurations. Our results suggest that the advantage of using this method to determine β is that the asymptotic quantity $\overline{G}(t)$ is virtually independent of the system size in the early time region. Consequently, $\overline{G}(t)$ scales over a larger time interval than $W(t)$, and gives generally a much more accurate estimate of β even for relatively small systems. Using our best data for the larger system in $d = 2 + 1$, we obtain our most accurate estimate of β:

$$\beta(3) = 0.250 \pm 0.005.$$

We can also use G to find the parallel correlation length $\xi_{\parallel}(t)$ by defining it to be proportional to the minimum distance r where $G(\boldsymbol{r}, t)$ reaches its asymptotic value $\overline{G}(t)$. We tested this by defining a radius $r_c(t)$ as $G(r_c(t), t) = c\overline{G}(t)$ where $c < 1$ is a constant. Then, we expect that $r_c(t) \sim \xi_{\parallel}(t) \sim t^{1/z}$, independently of the value of c. We calculated $r_c(t)$ for $c = 0.5, 0.9$ and 0.95 in $d = 1 + 1$, and for $c = 0.9$ in $d = 2 + 1$. In figure 6 we display typical results for $d = 1 + 1$ and $d = 2 + 1$. Fitting straight lines to this data we obtain the estimates $1/z = 0.668 \pm 0.009$ and 0.625 ± 0.015, respectively, which agree well with our other results. Combining our best estimates for the exponents in $d = 2 + 1$, $\chi = 0.4$ and $z = 1.6$ we show in figure 7 a check of the scaling form of equation (1.2) and the agreement is satisfactory.

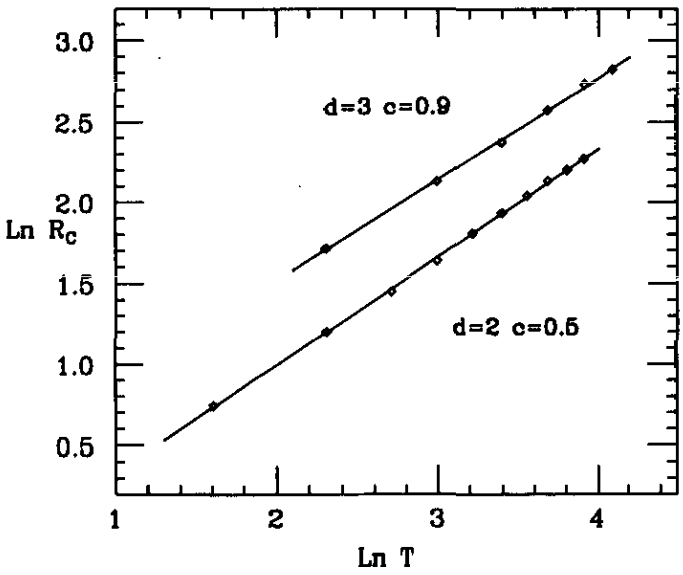

Figure 6. $r_c(t) \sim \xi_{\parallel}(t)$ against time for $d = 1 + 1$ and $d = 2 + 1$, as obtained from the height correlation function. The slopes of these curves give an estimate of $1/z$.

Finally, we note that one can define another time correlation function $\hat{G}(t)$ in the *saturated regime* such that

$$\hat{G}(t) \equiv \langle [\hat{h}(\boldsymbol{r}, t_0 + t) - \hat{h}(\boldsymbol{r}, t_0)]^2 \rangle_r \tag{2.9}$$

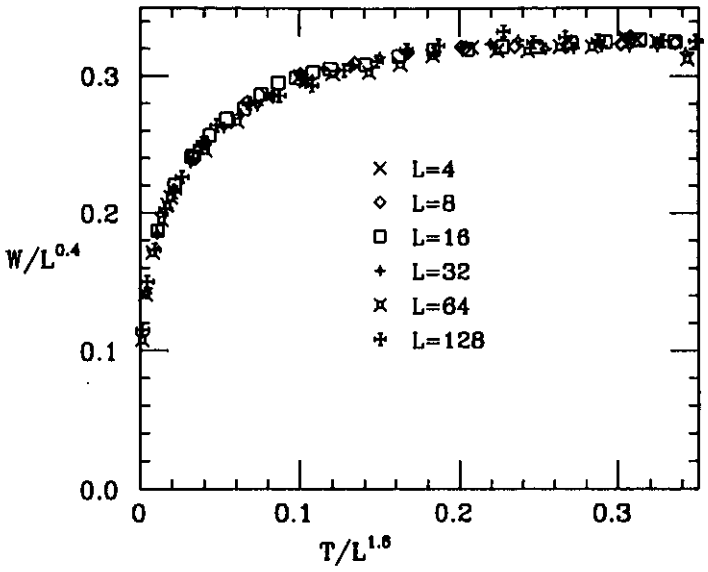

Figure 7. Scaling plot in $d = 2+1$ of $W(t,L)/L^{0.4}$ against $t/L^{1.6}$.

where $t_0 \gg L^z$. We then expect that $\hat{G}(t) \sim t^{2\beta}$, as proposed by Kardar *et al* (1986). For purposes of testing, we computed $\hat{G}(t)$ for a system of the size $L = 512$, in $d = 1+1$ and obtained $\beta = 0.332 \pm 0.006$ for $4 < t < 32$.

2.1.4. Finite size behaviour of the correlation function. To understand our numerical results better, according to which the asymptotic value $\overline{G}(t)$ of the correlation function yields consistently better results for the time exponent β than $W(t)$, we have to examine these two quantities in more detail. From the definition of G we obtain

$$G(\boldsymbol{r},t) = \langle[\hat{h}(\boldsymbol{r},t) - \hat{h}(0,t)]^2\rangle = 2W^2(t) - 2\langle\hat{h}(0,t)\hat{h}(\boldsymbol{r},t)\rangle \tag{2.10}$$

where $\hat{h}(x,t) = h(x,t) - \bar{h}(t)$. Then, for a system of infinite size $W^2(t) = \overline{G}(t)/2$. However, for finite systems we expect $W^2(t)$ and $\overline{G}(t)/2$ to behave differently (Kim 1989, Forrest *et al* 1990). Using the result $\langle\int \hat{h}(0,t)\hat{h}(\boldsymbol{r},t)\mathrm{d}\boldsymbol{r}\rangle = 0$, it follows that

$$W^2(t) = \frac{1}{2L^{d_s}} \int \mathrm{d}\boldsymbol{r}\, G(\boldsymbol{r},t). \tag{2.11}$$

The difference between $W^2(t)$ and $\overline{G}(t)$ can be obtained approximately from the known scaling behaviour of $G(\boldsymbol{r},t)$. Using equation (2.7) for early times, we can estimate the integral (2.11) by

$$W^2(t) = \frac{1}{2L^{d_s}} \int \mathrm{d}\boldsymbol{r}\, G(\boldsymbol{r},t) \approx \frac{1}{2}\overline{G}(t)\left[1 - O(1)\left(\frac{t^{1/z}}{L}\right)^{d_s}\right]. \tag{2.12}$$

This result means that when we use the scaling form of $W^2(t)$ to extract β, we obtain an *effective* exponent between $1 \ll t^{1/z} \ll L$ given by

$$\beta_{\mathrm{eff}}(t) \approx \beta - C\left(\frac{t^{1/z}}{L}\right)^{d_s} \tag{2.13}$$

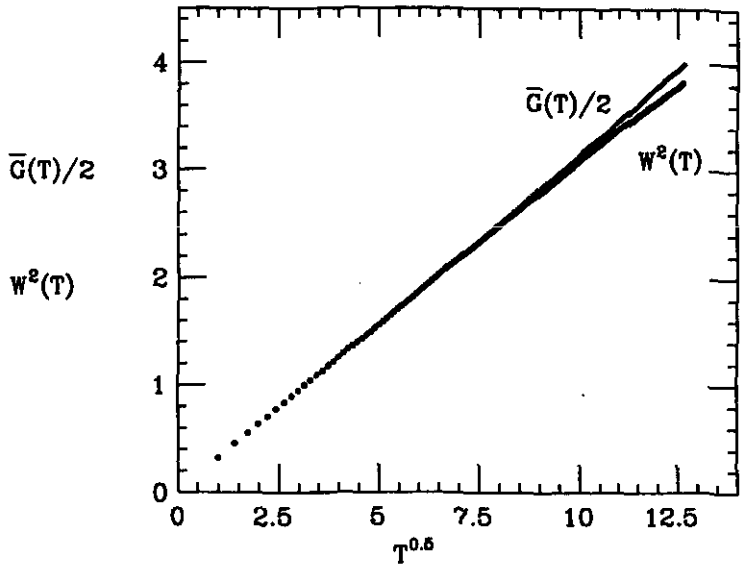

Figure 8. Time dependence of the height correlation function $\overline{G}(t)/2(L = 256)$ and the surface width $W^2(t)(L = 512)$ in $d = 2 + 1$. Even for larger systems, using $W(t)$ tends to *underestimate* the true exponent β.

where $C > 0$ is a constant. These results indicate that using the interface width always tends to *underestimate* the true value of the exponent β.

In figure 8 we show a comparison between $\overline{G}(t)/2$ and $W^2(t)$ plotted against the expected power law behaviour $t^{1/2}$, for systems of the sizes $L = 256$ and 512, respectively, in $d = 2 + 1$. There is a clear downward curvature in $W^2(t)$ at later times, because of the finite size effect.

2.2. Irrelevant variables and crossover effects during growth

In the previous section, we have seen that the GRSOS model with the minimum height restriction $N = 1$ seems to yield well defined and accurate values of the growth exponents. In fact, the results seem to suggest that, if the model is described by the strong coupling regime of the KPZ growth equation, the value of the effective coupling constant must be large.

In order to address this question, it is then important to determine which features in the GRSOS model are responsible for the robust numerical behaviour observed in the simulations. To this end, we have performed additional simulations of the model by changing the growth restriction parameter N, as well as employing some of the standard numerical tricks such as the noise reduction method which is believed to reduce the intrinsic width in some growth models. This allows us to study the effect of irrelevant variables and crossover behaviour in the GRSOS model, and also clarify the relation of the model to the continuum KPZ equation.

2.2.1. Effect of the height restriction parameter. The height constraint parameter N, which directly controls the interface width, has a strong influence on the growth of the columns. We performed simulations for various values of N in $d = 1 + 1$ and $d = 2 + 1$ to study this systematically, and in figure 9 we show a comparison of the calculated width W for $N = 1$ and $N = 4$ in $d = 2 + 1$. While the $N = 1$ curve

rapidly approaches its asymptotic behaviour, for $N = 4$ there is a long initial region dominated by the random deposition exponent $\beta = 1/2$, followed by a slow crossover towards the same asymptotic behaviour as in the case $N = 1$. This means that with increasing value of N, a typically *larger* values of the effective exponent β_{eff} are obtained. For example, using the data shown in figure 9 we obtain $\beta = 0.255 \pm 0.008$, which is already somewhat larger than our conjectured result $\beta = 1/4$. Additional simulations in $d = 1 + 1$ gave very similar results. For any $N < \infty$, the value of N only changes the short wavelength fluctuations which should be irrelevant as far as the scaling exponents are concerned. However, the value of N has drastic effects for the *effective* exponents obtained from simulations of smaller systems, where it becomes difficult to reach the asymptotic behaviour.

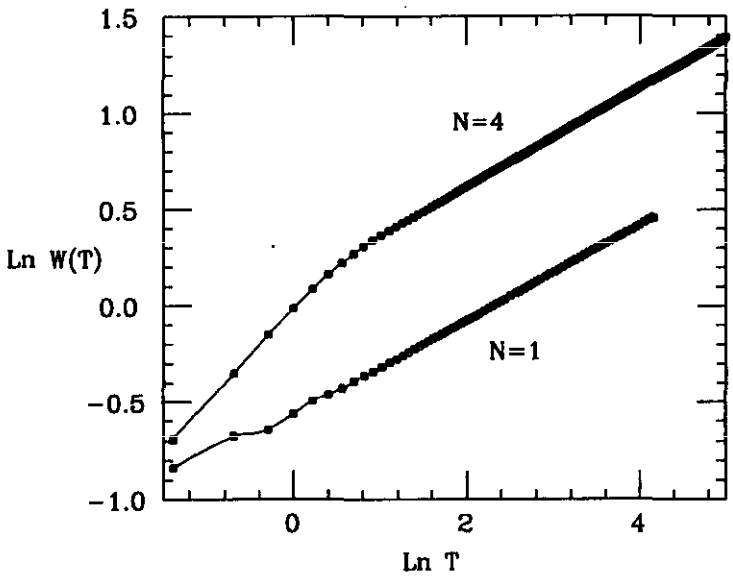

Figure 9. Effect of the height restriction parameter to the interface width in $d = 2 + 1$. For higher values of N, there is a pronounced early time random deposition regime with $\beta = 1/2$, followed by a slow crossover. System size used is $L = 512$.

2.2.2. Effect of the noise reduction method. Wolf and Kertész (WK) have recently introduced a method to reduce the short wavelength fluctuations in the Eden growth model (Wolf and Kertész 1987, Kertész and Wolf 1988). In their *noise reduction method*, a counter is assigned for each site on the surface. Each time a successful attempt is made to grow on a given site, its counter is increased by one instead of growing. Actual growth (by a discrete step) takes place only after the value of the counter reaches a preassigned value M, where M is called the noise reduction parameter. This method was used by WK to estimate growth exponents for the Eden model, using the idea that as noise reduction is turned on, the intrinsic width is suppressed and the dynamic scaling shows up already for relatively small system sizes. The noise reduction method clearly succeeds in reducing the intrinsic width; however, by the same token it may increase effective surface tension and parallel correlations in the GRSOS model, thus *reducing* the value of the KPZ coupling constant g and leading to complicated crossover behaviour (Wolf and Kertész 1989, Kim and Kosterlitz 1989b).

We investigated the effect of the noise reduction method on the GRSOS model by applying the algorithm in a straightforward manner during growth. In figure 4 we show for comparison the effect of increasing M from its default value ($M = 1$) up to $M = 8$ in $d = 2 + 1$. The surface width is clearly reduced, but instead of showing the expected scaling behaviour with $\chi = 0.4$, the curves for higher M do not appear to be in the scaling regime for the system sizes studied. In figure 10, we show a series of curves in $d = 1 + 1$ with increasing value of M, up to $M = 8$. A detailed examination of the early time behaviour reveals pronounced oscillations of the surface width, as increasing M tends to emphasize layerwise growth. This also yields an effective value of β which, for a given time interval, *decreases* with increasing value of M. The curves of figure 10 are due to competition between a crossover from the surface tension dominated regime at short times towards asymptopia and saturation due to finite size at long times.

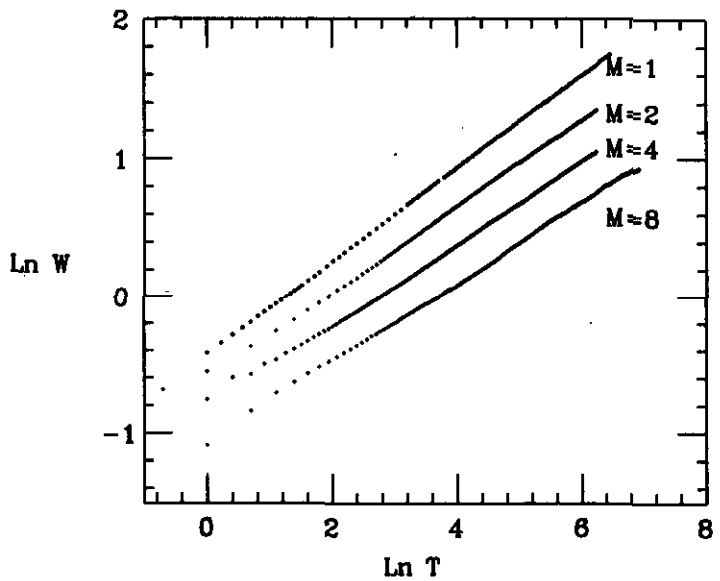

Figure 10. Effect of the noise reduction parameter M to the width in $d = 1 + 1$ for $L = 512$.

The effect of the noise reduction parameter is readily understood in the limit $N \to \infty$, i.e. for the random deposition model. Namely, the surface width trivially satisfies $W^2(M = 1, t) = MW^2(M, t/M)$ where the scaling of time by M is exact. Such simple scaling has also been used in the context of other growth models (Wolf and Kertész 1989). However, in the GRSOS and other models, where nonlinear effects such as lateral growth are present there is no reason why this scaling should hold. In fact, we calculated the saturated surface width as a function of M in $d = 1 + 1$ and obtained $W(M, t = \infty) \sim 1/M^{0.39}$, instead of the inverse square root behaviour. This, together with the increasing correlations parallel to the substrate, makes it difficult to reliably estimate growth exponents using the noise reduction method in the GRSOS model.

3. Generalized GRSOS model with deposition and evaporation

Our simulation results of the scaling exponents strongly indicate the presence of nonlinear terms in the GRSOS model, as described by the KPZ equation. The coefficient λ *in the* KPZ *equation describing lateral growth is the curvature of the inclination* dependent local growth velocity (Krug 1989). Recently, this quantity has been calculated numerically for the GRSOS model revealing that λ is indeed non-zero, and negative (Kim 1989, Krug and Spohn 1990a, Kim *et al* 1990, Huse *et al* 1990). As we mentioned in section 2, the same conclusion can be obtained from local step growth arguments, leading to the conclusion that the minimum height constraint $N = 1$ *maximizes* $|\lambda|$ in the model, leading to a large KPZ coupling constant g. This conclusion is also supported by recent simulations of the finite temperature GRSOS model, where λ depends on a temperature-like parameter (Amar and Family 1990a).

The effect of the lateral nonlinearity and the effective surface tension term in the KPZ equation can be further clarified by generalizing the GRSOS model to allow the evaporation of particles with the same height constraint N. It can then be shown that the lateral growth rate becomes proportional to the difference between the evaporation and deposition rates (Kim 1989). Thus, for the pure deposition model of section 2, $\lambda < 0$, while for the *symmetric case* where the two rates are equal, λ should vanish. Another way of seeing this is that in the latter case, the reflection symmetry $h \to -h$ is restored and the $\lambda(\nabla h)^2$ term must disappear (Plischke *et al* 1987).

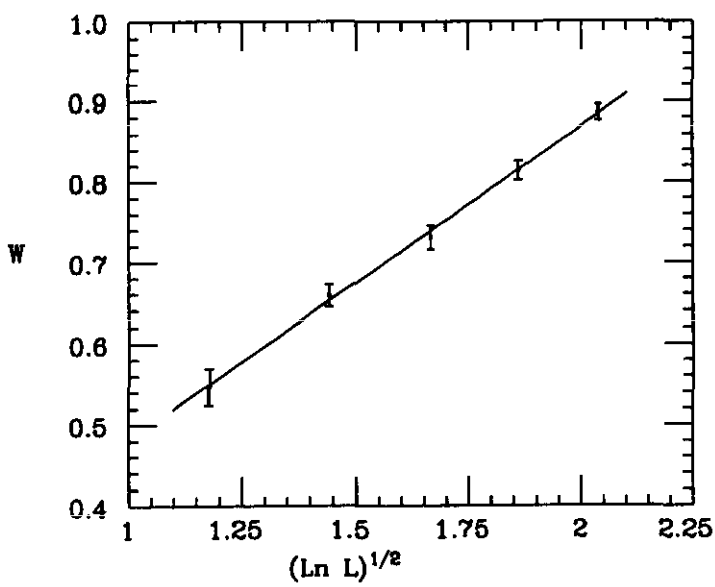

Figure 11. Interface width of the symmetric GRSOS deposition and evaporation model, for which $W(L) \sim \sqrt{\ln L}$ in $d = 2 + 1$ in the saturated regime. This result indicates that for the symmetric model $\lambda = 0$.

To verify this, we performed additional simulations for the symmetric adsorption–desorption case (without any explicit diffusion events) in $d = 1 + 1$ and $d = 2 + 1$. Using the surface width in the regime (ii), we obtained for the former case the result $\beta = 0.245 \pm 0.008$, which agrees well with the exact result of $1/4$ for the linear equation. Moreover, in the saturated regime the interface should be logarithmically rough in

$d = 2 + 1$ if $\lambda \equiv 0$. In figure 11 we show $W(L)$ plotted against $(\ln L)^{1/2}$ verifying this result. These results indicate, that *both* λ *and* ν are non-zero for the GRSOS deposition model suggesting that the strong coupling regime of the KPZ equation may be described by our model. The $\lambda = 0$ results indicate that there is no remnant of an equilibrium roughening transition in the GRSOS model so the discrete column heights of the simulations play little part, at least in the absence of noise reduction.

4. Summary and conclusions

In this work, we have presented a detailed numerical study of growth in the RSOS model. In particular, we have done systematic comparisons between various physical quantities, which can, in principle, be used to determined the scaling exponents for a given system size. Since quantities such as the interface width $W(t)$ and the correlation functions $\overline{G}(t)$ defined in section 2.1.3 are subject to unknown finite size effects, it is important to use the quantity which is least susceptible to these. In analogy with critical phenomena, it is natural to expect that $\overline{G}(t)$, which contains only the important long wavelength fluctuations, would suffer less from these finite size corrections than $W(t)$ which contains fluctuations from all length scales. Our results indeed indicate (see figure 8) that when limited system sizes are used, the spatially averaged correlation function $\overline{G}(t)$ yields the most reliable results for β. Moreover, using the surface width $W(t)$ instead tends to underestimate the true value of β which may explain some of the results appearing in the literature. We have also used the saturation of the interface fluctuation to determine χ independently. Our best data for both exponents then leads us to conjecture new, dimension-dependent scaling exponents as given by equation (1.6).

Our results indicate that the GRSOS model is particularly useful in studying the role of possible crossover phenomena in discrete growth models. By relaxing the height constraint, and introducing noise reduction we can see an immediate deterioration in the quality of the observed scaling regime in the model. In particular, the effect of increasing the noise reduction parameter M is highly non-trivial, and leads to systematically smaller values of β. Thus, the GRSOS model with $N = 1$ *and* without noise reduction seems to be 'optimal' for numerical studies.

Direct numerical integrations of the KPZ equation in $d = 2 + 1$ dimensions have given scaling exponents which are distinctly below our conjecture (Chakrabarti and Toral 1989, Guo *et al* 1990), but a recent study of Amar and Family (1990b) shows strong crossover effects for small g and the value of β close to 0.25 in the late time regime for large g. However, the relation of the discrete growth models to the continuum KPZ equation remains unclear. Moreover, there exists a very large scale simulation of a hypercube stacking model (Forrest and Tang 1990), which gives a slightly smaller value of $\beta = 0.240 \pm 0.001$ in $d = 2+1$, and also a smaller $\beta(4) = 0.180 \pm 0.005$. This simulation was performed running a parallelized code with very large system sizes up to $L = 11520$ in $d = 2+1$. The small error bar for $\beta(3)$, would seem to exclude our conjectured value of $1/4$. However, the hypercube stacking model can be mapped into an RSOS model on three triangular sublattices, with non-trivial next-nearest-neighbour height constraints in the sublattice (Kim and Kosterlitz 1990, Forrest *et al* 1990). As we have seen in this work, these additional interactions may introduce non-trivial crossover effects, which are difficult to quantify in estimating the exponents. Finally, we would like to mention that, although the exponents of equation (1.6) have recently

been shown to follow from a Flory type of argument (Hentschel and Family 1991), we believe that additional analytic work, and large scale simulations of well understood models are called for in order to reliably determine the possible universal values of the scaling exponents.

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