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COMMENT

Absence of non-trivial asymptotic scaling in the Kashchiev model of polynuclear growth

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Abstract. In this brief comment we show that, contrary to previous claims (Bartelt and Evans), the asymptotic behaviour of the Kashchiev model of polynuclear growth is trivial in all spatial dimensions, and therefore lies outside the Kardar–Parisi–Zhang universality class.

Within the field of non-equilibrium interface growth, one of the central issues is the existence of dynamical scaling and associated universality classes [1, 2]. The simplest quantity which may exhibit such scaling is the interface width $w(L, t)$. For a system of lateral size L, the scaling form for w may be written as $w(t) \sim L^{\chi} f(t/L^{z})$ for times t larger than some microscopic time scale. In the limit of infinite L, one then expects the asymptotic time evolution of the width to follow $w \sim t^{\beta}$ where $\beta = \chi/z$. The determination of the exponents z and χ represents a primary objective within this field. One of the most popular models of interface growth is due to Kardar, Parisi and Zhang (KPZ) [3], and through a concerted effort (mostly on the numerical front), there now exist rather precise estimates for the exponents in low spatial dimensions (see, for example, [4]). An analytic derivation of these exponents represents an outstanding theoretical challenge.

In a recent paper [5], Bartelt and Evans (BE) presented an analysis of the Kashchiev model [6], which is closely related to polynuclear growth (PNG) models [7–9]. This model has the unusual feature of being exactly solvable in the sense that the average interface height $h(t)$ and the width $w(t)$ may be expressed in terms of a closed set of coupled integral equations. A numerical study of these equations was undertaken by BE. From their results, they concluded that the interface width of the Kashchiev model showed non-trivial asymptotic scaling which were consistent (within numerical error) with KPZ universality. They also raised the possibility that an exact asymptotic analysis of this model may enable one to determine the upper critical dimension (above which $\beta = 0$) of the KPZ model.

To investigate such a possibility was our motivation for a closer analysis of the Kashchiev model. Our results (to be presented below) convincingly demonstrate that the asymptotic behaviour of the Kashchiev model is trivial in the sense that the growth exponent $\beta(d) = \frac{1}{2}$ for all d. This model therefore lies outside the KPZ universality class. Our presentation shall henceforth be brief, and we refer the reader to [5] for details of the formulation of the Kashchiev model.

The central quantity in the Kashchiev model is the function $\theta_i(t)$ which represents the fraction of layer i which is covered with deposited material at time t. The form of $\theta_1(t)$ is known exactly, and the higher functions $\theta_{i>1}(t)$ may be generated iteratively via the integral equations

$$\theta_{i+1}(t) = \int_0^t \mathrm{d}t' \, \{1 - \exp[-(t-t')^{d+1}]\} \frac{\mathrm{d}\theta_i(t')}{\mathrm{d}t'} \, . \tag{1}$$

In terms of these layer coverages θ_i, the average height may be expressed as

$$h(t) = \sum_{i=1}^{\infty} \theta_i(t) \tag{2}$$

and the mean square width $W(t) \equiv w(t)^2$ takes the form

$$W(t) = \sum_{i=1}^{\infty} (2i-1)\theta_i(t) - h(t)^2 \, . \tag{3}$$

(These expressions differ in a minor, inessential, way from those of BE. Note also that our unit of time is exactly half that used by BE.)

The numerical analysis of BE seems to have proceeded by iteratively solving the set of integral equations for a given number of the functions $\theta_i(t)$, and then summing these functions in order to determine $h(t)$ and $W(t)$. This method will fail for large times as one is forced to calculate an increasingly large number of layer coverages to ensure numerical precision. The predictions of asymptotic scaling in accord with KPZ scaling was made on the basis of calculating the first five layer coverages, which is insufficient to investigate the true asymptotic regime.

A simple way around this problem is to sum the recursion relation (1) over *all* the layer coverages θ_i with an appropriate weight such that one derives closed integral equations for $h(t)$ and $W(t)$. One then has no numerical barriers in probing the deep asymptotic regime. The equation for the mean height, written in terms of the deviation from linear growth $\Delta(t) \equiv h(t) - v(d)t$, takes the form

$$\int_0^t \mathrm{d}t' \, \frac{\mathrm{d}\Delta(t')}{\mathrm{d}t'} \exp[-(t-t')^{d+1}] = 1 - \exp(-t^{d+1}) - v(d) \int_0^t \mathrm{d}t \, \exp(-t'^{d+1}) \, . \tag{4}$$

The d-dependent velocity is given by $v(d)^{-1} = \Gamma((d+2)/(d+1))$, where $\Gamma(z)$ is the gamma function [10]. For the mean square width, we have

$$\int_0^t \mathrm{d}t' \, \frac{\mathrm{d}W(t')}{\mathrm{d}t'} \exp[-(t-t')^{d+1}] = 2h(t) - \int_0^t \mathrm{d}t' \, \frac{\mathrm{d}h(t')}{\mathrm{d}t'} [1 + 2h(t')] \exp[-(t-t')^{d+1}] \, . \tag{5}$$

The above equations are of the Volterra type, and we may therefore use relatively simple techniques for their numerical solution. More precisely, we use a uniform grid for the discretization, along with a trapezoidal rule for the integration [11]. The discrete time step used here is $\delta t = 0.001$, yielding results with a precision of six significant figures. We should emphasize that on reducing the time step further, the precision can be systematically improved.

The reason for studying the deviation from linear growth of $h(t)$, via the function $\Delta(t)$, is that one might expect on simple scaling grounds that $\Delta(t) \sim t^{\beta}$. In figure 1 we present our results for $\mathrm{d}\Delta(t)/\mathrm{d}t$, for $d = 1, 2$ and 3. The function becomes increasingly oscillatory for higher dimensions. The decay of the envelope of the oscillations is exponential after some transient period (which grows slowly with increasing dimension). We have determined the decay rate $\lambda(d)$ for the exponential decay with high precision as a function of d. The inset in figure 1 shows the d dependence of λ on a log–linear scale. In figure 2,

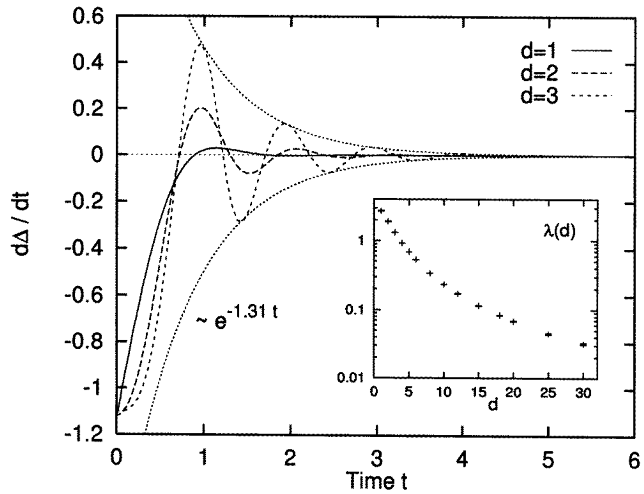

Figure 1. The time derivative of the deviation of $h(t)$ from linear growth, $\mathrm{d}\Delta(t)/\,\mathrm{d}t$, as a function of t, for $d = 1, 2, 3$. This data comes from numerical integration of (4). The exponential decay of the envelope of oscillations is illustrated for the $d = 3$ curve. The inset shows the d dependence of the decay rate λ on a log–linear scale.

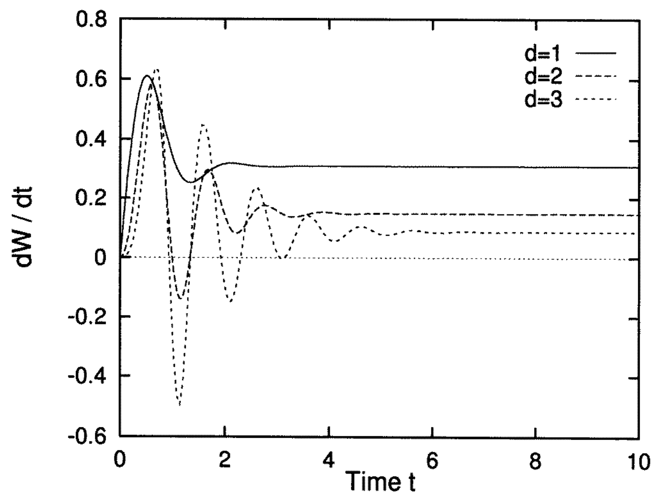

Figure 2. The time derivative of the mean square fluctuations, $\mathrm{d}W(t)/\,\mathrm{d}t$, as a function of t, for $d = 1, 2, 3$. This data comes from simultaneous numerical integration of (4) and (5).

we show the evolution of the time derivative of $W(t)$ for $d = 1, 2$ and 3. Results for higher dimensions are qualitatively similar. Again we see that the pre-asymptotic behaviour is increasingly oscillatory as one increases the dimension d. The asymptotic behaviour, however, is purely constant, implying that $W(t) \sim b(d)\,t$, and hence that $\beta = \frac{1}{2}$ for all d. The full dimensional dependence of $b(d)$ is plotted in figure 3. One may also study the pre-asymptotic corrections to this linear form for $W(t)$. These oscillatory corrections are also found to have an exponentially decaying envelope, with a decay rate $\tilde{\lambda}(d)$ which satisfies the relation $\lambda(d) \simeq 1.14(2)\tilde{\lambda}(d)$. These results show convincingly that the asymptotic

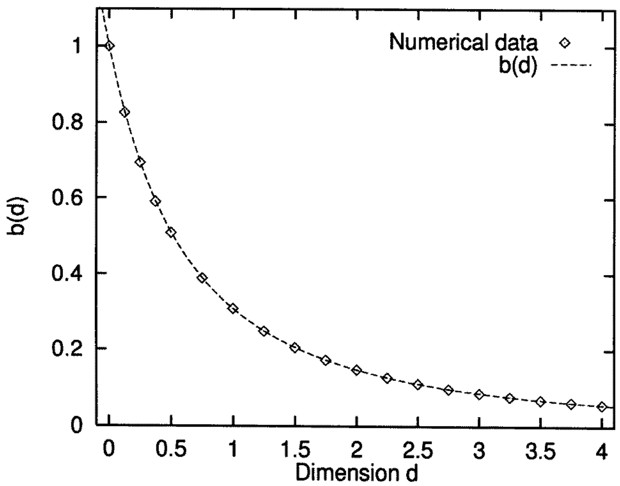

Figure 3. The d dependence of the amplitude $b(d)$, from the asymptotic relation $\mathrm{d}W(t)/\,\mathrm{d}t \sim b(d)$. The broken curve is the relation given in (6), whilst the data points are from numerical integration of (5).

properties of the Kashchiev model are trivial; i.e. the mean height relaxes exponentially fast to linear growth, and the interface width evolves as the square root of time.

As a powerful check on the numerical work, we may solve the integral equation for the mean square width $W(t)$ in the deep asymptotic regime by making the ansatz $\mathrm{d}W(t)/\,\mathrm{d}t \sim b(d)$, and taking $h(t) \sim v(d)\,t$, with $v(d)$ defined previously. Inserting these forms into (5) and taking $t \to \infty$ allows one to extract the prefactor $b(d)$. Explicitly one finds

$$b(d) = v(d)\left\{\Gamma\left(\frac{d+3}{d+1}\right)v(d)^2 - 1\right\}. \tag{6}$$

This functional form is plotted against the numerical results in figure 3. Excellent agreement is obtained, indicating both the correctness of the above ansatz, and the high precision of the numerical work.

For comparison with the above results, we mention that the above equations may be easily solved in the limits of $d = 0$ and $d = \infty$ by use of Laplace transform methods. One finds for $d = 0$, that $h(t) = t$ and $W(t) = t$ exactly. For $d = \infty$ one has layer-by-layer growth described by $h(t) = n, n < t < n+1$ and $W(t) = 0$ exactly. The infinite d results are consistent with (i) the increasingly oscillatory behaviour found numerically for larger values of d (a trend towards layer-by-layer growth), and with (ii) $b(d)$ vanishing monotonically for large d.

Finally, we illustrate the misinterpretation of the data that led BE to conclude that $W(t)$ had KPZ-type scaling. Their conclusions arose from a plot of $W(t)$ versus $h(t)$. Since their data is not in the asymptotic regime, such a plot is potentially misleading as $h(t)$ still has appreciable deviations from linear growth. In figure 4, we present a linear plot of $W(t)$ versus $h(t)$ for $d = 1, 2$ and 3 for longer times than obtained by BE (cf figure 4 in [5].) It is seen that the relationship between $W(t)$ and $h(t)$ eventually becomes linear, in agreement with the scaling forms $h(t) \sim v(d)\,t$ and $W(t) \sim b(d)\,t$.

We conclude by remarking that models belonging to the PNG class are certainly worthy of study, as more realistic versions are known to exhibit KPZ scaling [8, 9]. However,

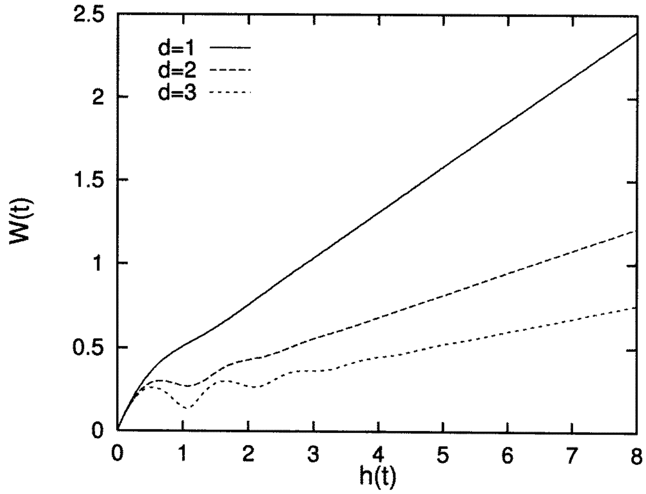

Figure 4. A plot of the mean square fluctuations $W(t)$ versus the average height $h(t)$, for $d = 1, 2, 3$.

any analytic treatment must be based on a less mean-field-like formulation than that of the Kashchiev model. It is of interest to determine precisely where the crucial mean-field assumption enters into the Kashchiev model, and whether it is possible to relax this assumption without making the model analytically intractable.

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