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LETTER TO THE EDITOR

Morphology of the interfacial patterns growing from unstable initial states in crystal growth models

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Abstract. Using the Walsh-Fourier transform of the interface function we introduce a new method for the analysis of the morphology of the complex interfacial patterns evolving with time on discrete lattices in a wide class of physical systems including crystal growth models. For the crystal growth models we also generalise an old technique for characterising the interfacial patterns on small length scales to patterns evolving from initial states far from equilibrium.

Formation and growth of fractal patterns (Stanley and Ostrowsky 1985) as well as non-fractal patterns (Langer 1980) in physical systems has become one of the main fields of interdisciplinary research during the last few years. The growth of the domains of up (or down) spins in an Ising model following an instantaneous quench from a very high temperature T_h to a low temperature T_l below the coexistence curve is a prototype example of freely equilibrating model systems evolving from unstable initial states where the relevant degrees of freedom are random (Gunton *et al* 1983). Except for the average linear domain size $R(t)$ and the scaling form of the structure function very little attention has been paid so far to the detailed morphology of the interfacial structure of such growing patterns. The growing surface profile of the Eden model (Plischke and Racz 1985, Kardar *et al* 1986, Zabolitzky and Stauffer 1986, Hirsch and Wolf 1986, Wolf and Kertész 1987) and that of the interfaces in directional solidification (Langer 1980) and in the Hele-Shaw cell (Bensimon *et al* 1986) has provided at least some insight into the morphology of some growing interfacial patterns. The main aim of this letter is to introduce two methods of analysing the morphology of interfacial patterns; while one of the methods characterises the global structures of the interfaces the other characterises the same patterns on short length scales. Most of our discussions will be based on the solid-on-solid (SOS) model as an example. Since SOS type models have been very successful in the study of crystal growth (Gilmer 1980) we believe that the techniques introduced in this letter will provide new tools for the investigation of the *shape* of more complex and more realistic systems.

Since neither 'droplets' of opposite spins nor 'overhangs' are allowed in the SOS model, the interface separating the 'up' spins from the 'down' spins can be represented as a single-valued function $z = f(i)$, where $i = 1, \ldots, N$ is the coordinate labelling the lattice sites in the $(d-1)$-dimensional hyperplane transverse to the z direction. The

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effective Hamiltonian for the SOS model in d dimensions is given by (Muller-Krumbhaar 1978)

$$\mathcal{H} = JL^{d-1} + (J/2)\sum_{\langle ij \rangle} |f(i) - f(j)| \tag{1}$$

where the sum $\langle ij \rangle$ denotes a sum over nearest-neighbour columns i and j. It is straightforward to verify that the ground state of the SOS model corresponds to a flat smooth interface, i.e. $f(i) =$ constant for all i. From now onwards, we shall focus our attention only on $d = 2$ and denote the direction perpendicular to the z direction by x. It is well known that for the two-dimensional SOS model the roughening temperature $T_R = 0$.

Our Monte Carlo algorithm for studying the dynamical evolution of the SOS model is analogous to the Glauber single spin-flip dynamics rather than Kawasaki spin-exchange dynamics. Therefore $\Sigma f(i)$ is not conserved during the dynamical evolution of the SOS model. The initial random configuration $f(i)$ $(0 \leq f(i) \leq M$ for $1 \leq i \leq N)$ is created using a random number generator. Obviously such a configuration is very far from the equilibrium configuration corresponding to a low temperature T. Let us assume that the spins below the interface are all 'up' and those above are all 'down'. A periodic boundary condition is applied along the x direction so that $f(N+1) = f(1)$. Then 'flipping' an Ising spin at $i = k$ just below the interface is equivalent to reducing the height $f(k)$ by unity. Similarly, 'flipping' an Ising spin at $i = k$ just above the interface is equivalent to increasing the height $f(k)$ by unity. Note that since no island is allowed in the SOS model, only the spins just above and just below the interface are allowed to flip. The Monte Carlo scheme for updating the variables $f(i)$ is very similar to the usual Metropolis algorithm. If the proposed energy change ΔE is less than or equal to zero, then the flipping is carried out; otherwise the flipping is carried out with probability $\exp(-\Delta E/k_B T)$ (Swendsen 1977). Recently Stauffer and Jan (1987) have investigated a growth model where the interface is modelled by self-avoiding walks. A crucial difference is the possibility of lateral growth in that model which contributes a non-linear term to the differential equation describing the growth process. Moreover, unlike the SOS model, overhangs are allowed in that work.

Let us now analyse the morphology of the interface of the SOS model during its evolution with time. Two quantities which have received some attention in several related contexts in the past are the length $L(t)$ and the width $W(t)$ of the interface. Our results on the $L(t)$ and $W(t)$ of the SOS model and their physical interpretations will be reported elsewhere (Chowdhury 1987). In this letter we shall investigate two other features of the interface which have received very little attention so far in the literature.

An interface may be very 'regular' (not necessarily flat) or 'irregular' up to a certain extent. The question we pose now is: how 'irregular' or 'noisy' is an interface at a given instant of time t during its evolution? In the continuum theories (see, for example, Sarkar and Jensen (1987) and references therein) the Fourier transform of the interface function $f(x; t)$ is given by $f(x; t) = \Sigma\, c_k(t) \exp(ikx)$ where $c_k(t)$ is the amplitude of the kth plane wave 'mode' at time t. Therefore, the time evolution of the interface can be described in terms of the corresponding time evolution of the Fourier coefficients $c_k(t)$. The larger is the number of modes for which amplitude $c_k \neq 0$ the noisier is the interface.

Let us now generalise the Fourier transform method appropriately for the discrete model (1). Since computer simulations as well as other numerical investigations are

almost always carried out on a discrete lattice, it is more convenient to use the Walsh-Fourier transform where the exponential functions $\exp(ikx)$ are replaced by the Walsh functions $D_k(x)$ (Harmuth 1972, Lord and Wilson 1984). Thus, the Walsh-Fourier transform of a function $f(x; t)$ is given by $f(x; t) = \Sigma\, a_k(t) D_k(x)$. Therefore the motion of the interface on a discrete lattice can be described in terms of the time evolution of the Walsh-Fourier coefficients $a_k(t)$. The Walsh functions $D_k(x)$ ($k = 0, 1, 2, \ldots$) are defined by

$$D_0(x) = 1 \qquad \text{for all } -\tfrac{1}{2} \leqslant x \leqslant \tfrac{1}{2}$$

$$D_1(x) = \operatorname{sgn}(\sin \pi x)$$

$$D_j(x) = \operatorname{sgn}(\cos j\pi x) \qquad \text{for } j = 2^n,\ n > 0$$

and

$$D_{m \oplus n}(x) = D_m(x) D_n(x)$$

where $m \oplus n$ denotes the operation modulo 2 addition of the binary representations of two integers m and n. For example, $D_7 = D_4 D_2 D_1$, $D_{12} = D_{10} D_6$.

The Walsh-Fourier transform is particularly useful for functions $f(x)$ which are stepwise discontinuous functions on 2^p intervals. Let us consider the SOS model with $N = 8$, so that the height of the interface $f(x)$ is a stepwise discontinuous function over the 2^p intervals with $p = 3$. The interval of x can be squeezed or stretched so that the eight points are within the interval between $-\frac{1}{2}$ and $\frac{1}{2}$. For example, the Walsh functions $D_k(x)$ for $k = 0, 1, 2, \ldots, 8$ are shown in figure 1.

We have monitored the coefficients $a_k(t)$ as a function of time t where t is measured in units of Monte Carlo steps (MCS) per site. Some of the $a_k(t)$ are shown in figure 2. Since the interface is perfectly flat only at $T = 0$, $|a_0| < 1$ at $t =$ any non-zero temperature. Therefore, at $T > 0$ the amplitude of not only the $k = 0$ mode but also that of several other modes remain non-zero at $t = \infty$. Moreover, since each of the

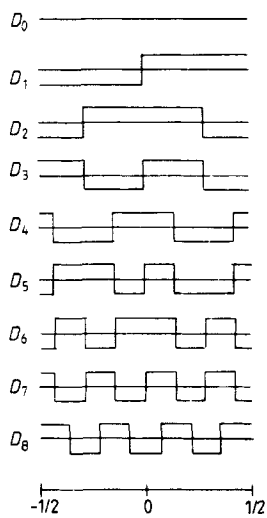

Figure 1. Walsh functions $D_k(x)$ for $k = 0$-8 within the interval $-\frac{1}{2} \leqslant x \leqslant \frac{1}{2}$. Note that there are some crucial differences between the Walsh functions and the corresponding sine functions.

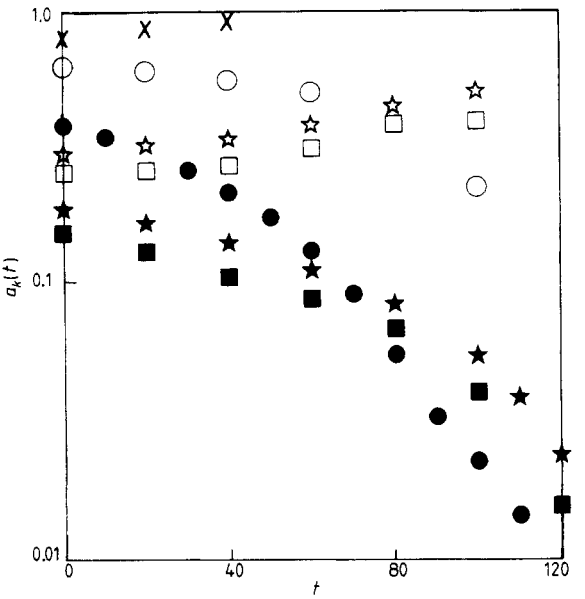

Figure 2. Walsh coefficients $a_k(t)$ for the SOS model at $T=0$ with $N=8$, plotted as a_0 (×), a_2 (●), a_3 (★) and a_4 (■) for $M=256$ and as a_2 (○), a_3 (☆) and a_4 (□) for $M=265$. Note that the heights were measured with respect to the mean height to obtain the data for $M=265$ and therefore the corresponding a_0 for $M=265$ were zero for all t.

Walsh functions is a superposition of several sine waves the relaxation of the Walsh coefficients is far from exponential. Indeed, the larger is k the smaller is the number of sinusoidal waves required to reproduce a Walsh function and the closer is the relaxation to exponential decay.

The method described above can also be generalised to three-dimensional systems. For the three-dimensional SOS model, for example, the two-dimensional interface $f(x, y; t)$ can be expanded in terms of the two-dimensional Walsh functions $D_{mn}(x, y) = D_m(x)D_n(y)$. Since our model does not incorporate bulk as well as surface diffusion processes it is not directly applicable to the relaxation of real crystal surfaces (Herring 1950, Mullins 1959, Maiya and Blakely 1967, Hoehne and Sizmann 1971, Martin and Perraillon 1977, Villain 1986, Selke 1987). However, we would like to emphasise that these are the drawbacks of the simple example we have chosen, namely the SOS model, and not a shortcoming of our basic technique.

The technique of the Walsh-Fourier transform can also be used for more complicated interfaces, for example, isolated droplets. For such interfaces although the interface $f(x)$ is a multiple-valued function of x, it *may* be a single-valued function of the angle ϑ in the (r, ϑ) coordinate system where the origin is at the 'centre of mass' of the interface. This property is utilised in the 'characterisation of shape by geometric signature waveform' (Kaye 1986). In such cases the angular resolution $\Delta\vartheta$ plays the role of the lattice constant in the SOS model. The interface function $r=f(\vartheta)$ can now be expanded in terms of the Walsh functions and the corresponding Walsh-Fourier coefficients describe the dynamical evolution of the interface.

Since the index k in $D_k(x)$ gives the number of zero crossings of D_k, the Walsh-Fourier analysis of the interface characterises the morphology on length scales beginning from the system size N down to the distance between the successive zero crossings

of $D_{k_{max}}(x)$ where $a_k = 0$ for all $k > k_{max}$. Let us now introduce a method for investigating only the *local* structure of the interface on a length scale of the order of a few lattice constants. For example, the morphology of the growing patterns in the kinetic Ising model can be described by monitoring the fraction of neighbouring lattice sites $C_n(t)$ with n dissimilar species. For a square lattice, an up (down) spin can have n down (up) spin neighbours, where n can vary from $n = 0$ to $n = 4$. So far as only the sites along the interface in the SOS model are concerned, n varies between 1 and 3. We shall consider only the interfacial sites on one side of the interface, i.e. either only the sites occupied by the 'up' spins or only by the 'down' spins. Accordingly, the interfacial sites can be in one of the three energy levels $(2n-4)J$, with $n = 1, 2, 3$. Similar ideas have been applied earlier (Jackson 1975) for characterising the equilibrium structure of the crystal-melt interface. In this letter we have generalised this approach to the study of the interfaces growing from initial states which are very far from equilibrium. We have monitored the fractions $C_n(t)$ as a function of time t (figure 3).

We conclude that the Walsh–Fourier coefficients yield a measure of the noise level in the interfacial pattern on discrete lattices. The relaxation of these *Walsh modes* is non-exponential. We have also demonstrated that the fractions $C_n(t)$ of *dissimilar neighbours* provide information on the local structure of the interfaces. Details of the results obtained by the applications of these techniques to various different models will be reported elsewhere (Chowdhury 1987).

It is my great pleasure to thank D Stauffer and J D Gunton for useful discussions.

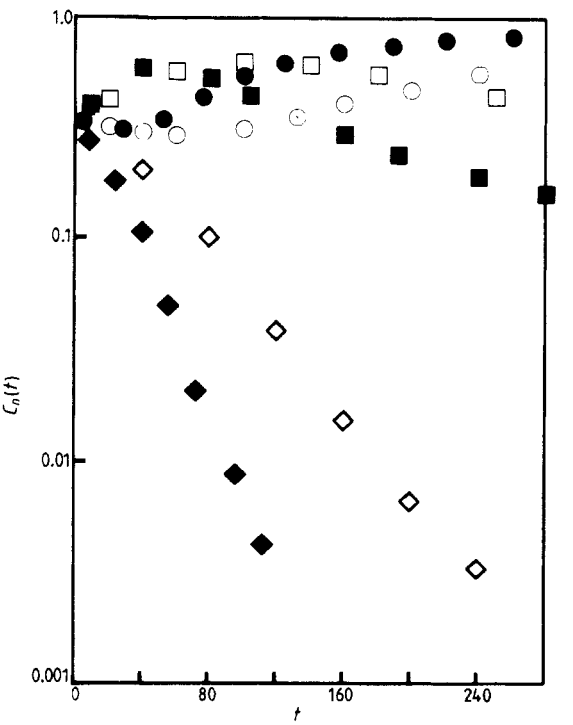

Figure 3. The fractions $C_n(t)$ for the SOS model at $T = 0$ with $N = 512$, plotted as C_1 (●), C_2 (■) and C_3 (◆) for $M = 128$ and as C_1 (○), C_2 (□) and C_3 (◇) for $M = 256$.

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