Dynamics of Gaussian interface models

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The relaxational dynamics of an initially flat $(d-1)$-dimensional interface in a d-dimensional system is modeled by the unweighted Gaussian model defined on a lattice and obeying Langevin dynamics. The interface width is calculated and is found to grow to its equilibrium value via three distinct limiting regimes, each containing different growth laws. Results are presented for $d=2$ and 3 with scaling properties and limiting behavior in full agreement with previous continuum models and simulations of kinetic growth models.

Over the last few years there has been a great deal of interest in the kinetics of aggregation and growth processes.[1] Some of the systems studied include granular aggregation,[2] solidification fronts[3] and vapor deposition.[4,5] Particular focus has been made on the way in which the interface, which separates the growing material from its environment, evolves in time. It is now believed, on the basis of numerical simulations and analytic work, that such an interface exhibits interesting scaling behavior.

In this Brief Report, we report on a systematic treatment of the dynamical behavior of a $(d-1)$-dimensional interface separating two phases in d dimensions. The two phases could be, for example, liquid-vapor phases (when $d=3$) or phases of opposite magnetization in an Ising ferromagnet. The interface is initially flat so that as time progresses its rms displacement (henceforth referred to as the interface width) increases until it relaxes into its equilibrium value which scales with the side length of the interface. This work differs from that of the first paragraph, in that it is concerned with systems relaxing to thermodynamic equilibrium, rather than a kinetic growth model relaxing to its steady state.

We first consider the case for $d=2$. For the equilibrium properties there exists an exactly solvable model that has been studied extensively, namely the planar spin-$\frac{1}{2}$ Ising model. In particular, Abraham has rigorously demonstrated[6] that when coarse graining to length scales of the order to the correlation length of the bulk phases, the equilibrium probability distribution $P_{\rm eq}$ of the heights h_j (where $h_j \in \mathbb{R}$ and $j \in \mathbb{Z} \cap [-L,L]$) of the renormalized interface can be expressed as

$$P_{\rm eq}\{h\} = Z^{-1}\exp(-\mathcal{H}\{h\}) , \tag{1}$$

where

$$\mathcal{H}\{h\} = \tfrac{1}{2}\sigma \sum_{j=-L}^{L-1} (h_{j+1}-h_j)^2 \tag{2}$$

and Z is the canonical partition function with respect to the "effective" Hamiltonian $\mathcal{H}$ (actually a free energy since internal degrees of freedom have been summed out). (1) and (2) are sometimes referred to as the *unweighted* or *massless Gaussian* model whose equilibrium properties are well known[7] for both $d=2$ and the $d=3$ model to be discussed later. σ is the effective interfacial tension of Fisher, Fisher, and Weeks,[8] given as $\sigma=\tau(0)+\tau''(0)$, where $\tau(\theta)$ is the microscopically derived interfacial tension for an Ising interface at angle θ from the lattice directions.[9] Note that the interface has length $2L$ in units of the bulk correlation length. Its boundary conditions imposed at the ends for all time are $h_L=h_{-L}=0$.

Since we wish to describe how a nonequilibrium configuration $\{h\}$ relaxes to equilibrium we use the Langevin equation of motion[10]

$$\frac{\partial h_j}{\partial t} = -\Gamma \frac{\partial \mathcal{H}\{h\}}{\partial h_j} + \eta_j(t) , \tag{3a}$$

where the Gaussian white noise $\eta_j(t)$ at site j has the usual correlation properties

$$\langle \eta_j(t)\rangle = 0, \quad \langle \eta_j(t)\eta_{j'}(t')\rangle = 2\Gamma\delta_{jj'}\delta(t-t') . \tag{3b}$$

The first term in the right-hand side of (3a) causes the interface to relax to the minimum of $\mathcal{H}$ while the noise $\eta_j(t)$ and the presence of Γ in both (3a) and (3b) ensures that the correct equilibrium distribution (1) is obtained in the static limit.[10] Insisting that the evolution of the interface obeys Langevin dynamics is the only approximation that has been made in our approach (provided that length scales are sufficiently large). From here on, everything we present is *exact* and *rigorous*.

By substituting (2) into (3a), one obtains a linear Langevin equation

$$\frac{\partial \underline{h}}{\partial t} = -\sigma\Gamma \underline{A}\,\underline{h} + \underline{\eta}(t) , \tag{4}$$

where $\underline{h}=(h_{-L+1},\ldots,h_{L-1})^T$, $\underline{\eta}(t)=(\eta_{-L+1}(t),\ldots,\eta_{L+1}(t))^T$, and $\underline{A}$ is a $(2L-1)\times(2L-1)$ tridiagonal matrix whose elements are

$$A_{ij} = \begin{cases} 2 \ \text{ for } i=j , \\ -1 \ \text{ for } |i-j|=1 , \\ 0 \ \text{ otherwise} . \end{cases} \tag{5}$$

It is quite straightforward to diagonalize $\underline{A}$ to obtain its eigenvalues

$$\lambda_q = 2(1-\cos q), \quad q=\frac{n\pi}{2L}, \quad n=1,2,\ldots,2L-1\,, \tag{6}$$

and the corresponding normalized eigenvectors.[11] It now follows that for each normal mode q

$$\frac{\partial \hat{h}_q}{\partial t} = -\sigma\Gamma\lambda_q \hat{h}_q + \hat{\eta}_q(t)\,, \tag{7a}$$

$$\langle \hat{\eta}_q(t)\rangle = 0, \quad \langle \hat{\eta}_q(t)\hat{\eta}_{q'}(t')\rangle = 2\Gamma\delta_{qq'}\delta(t-t')\,, \tag{7b}$$

where $\hat{h}_q$ and $\hat{\eta}_q(t)$ are normal coordinates.

Equations (7) constitute the well-known Langevin equation for a Brownian particle[12] of velocity $\hat{h}_q$ with a constant of friction equal to $\sigma\Gamma\lambda_q$. It is then standard to obtain the conditional probability distribution that the q normal coordinate is equal to $\hat{h}_q(t)$ at time t given that it is initially at $\hat{h}_q(0)$. This is done by deriving a Fokker-Planck equation from (7), following Uhlenbeck and Ornstein.[13] By insisting that the interface be initially flat $[\hat{h}_q(0)=0\ \forall q]$, it is now possible[11] to evaluate the *moment generating function* for moments of h_0

$$\langle \exp[ih_0(t)\phi]\rangle = \exp[-\alpha_L(t)\phi^2]\,, \tag{8}$$

where

$$\alpha_L(t) = \sum_{n=0}^{L-1} \frac{1-\exp\left\{-4\sigma\Gamma t\left[1-\cos\left[\frac{(2n+1)\pi}{2L}\right]\right]\right\}}{4\sigma L\left[1-\cos\left[\frac{(2n+1)\pi}{2L}\right]\right]}\,. \tag{9}$$

Clearly, $\langle h_0^2(t)\rangle = 2\alpha_L(t)$ so $\alpha_L(t)$ provides us with an expression for the *interface width squared*. Also, if one is considering an interface in a planar Ising model, one can obtain an expression for the magnetization profile.[11] This is done by first deriving the probability distribution that the interface height at $j=0$ passes through h_0, which is simply the inverse Fourier transform of the moment generating function. One can then use this to calculate the magnetization at position $(0,y)$ for time t, $m((0,y);t)$, which turns out to be

$$m((0,y);t) = m^*\Phi\{y[4\alpha_L(t)]^{-1/2}\}\,, \qquad \Phi(x) = \frac{2}{\sqrt{\pi}}\int_0^x \exp(-u^2)\,du \tag{10}$$

where m^* is the (equilibrium) spontaneous magnetization for the bulk Ising model. Obviously, this assumes local equilibrium on length scales smaller than the bulk correlation length. It should be stressed that within Langevin dynamics and for sufficiently large length scales, expression (10) provides us with a time-dependent generalization to the static result obtained by Abraham and Reed.[14]

It is interesting to note that Eq. (9) is remarkably similar to the analogous expression derived by Plischke, Rácz, and Liu[5] who were using Glauber[15] (as opposed to Langevin) dynamics on a different discrete model.

We now calculate $\alpha_L(t)$ for an interface of infinite extent. Using Abramowitz and Stegun[16] it can be shown that

$$\lim_{L\to\infty} \alpha_L(t) = \Gamma t e^{-4\sigma\Gamma t}[I_0(4\sigma\Gamma t) + I_1(4\sigma\Gamma t)]\,, \tag{11}$$

where I_0 and I_1 are modified Bessel functions. Their limiting behavior[16] gives

$$\lim_{L\to\infty} \alpha_L(t) \sim \begin{cases} \Gamma t & \text{for } t\to 0\,, \\ \left(\dfrac{\Gamma t}{2\pi\sigma}\right)^{1/2} & \text{for } t\to\infty\,. \end{cases} \tag{12}$$

Thus, an interface of infinite extent will thicken diffusively for initial times and then, for large times, the diffusive regime will break down into one of *slower* nondiffusive growth.

We next consider $\alpha_L(t)$ for a large but *finite* interface, for which (9) implies the following scaling behavior:

$$\alpha_L(t) \sim \frac{L}{\sigma} f\left(\frac{\sigma\Gamma t}{L^2}\right) \quad \text{for } L\to\infty,\ t\to\infty\,, \tag{13}$$

where

$$f(x) = \tfrac{1}{4}\left[1 - \frac{8}{\pi^2}\sum_{n=0}^{\infty}\frac{\exp[-\frac{1}{2}\pi^2(2n+1)^2 x]}{(2n+1)^2}\right]. \tag{14}$$

The limiting properties of $f(x)$ are

$$f(x) \sim \begin{cases} \left(\dfrac{x}{2\pi}\right)^{1/2} & \text{for } x\to 0\,, \\ \dfrac{1}{4} - \dfrac{2}{\pi^2}\exp(-\frac{1}{2}\pi^2 x) & \text{for } x\to\infty\,, \end{cases} \tag{15}$$

where the $x\to 0$ behavior was obtained using the Poisson summation formula. Note that this limit coincides exactly with the $t\to\infty$ case of expression (12). Hence, we have established three distinct (limiting) scaling regimes: $t\to 0$; $t\to\infty$ with $t/L^2\to 0$; and $t/L^2\to\infty$.

We now consider $d=3$. A three-dimensional version of (2) is

$$\mathcal{H}\{h\} = \tfrac{1}{2}\sigma \sum_{m=-L}^{L-1}\sum_{n=-L}^{L-1}[(h_{m+1,n}-h_{m,n})^2 + (h_{m,n+1}-h_{m,n})^2]\,, \tag{16}$$

with boundary conditions

$$h_{\pm L,n} = h_{m,\pm L} = 0\ \forall n,m \in \mathbb{Z}\cap[-L,L]\,.$$

This is the Weeks columnar model[17] and has been used to describe the equilibrium structure of liquid-vapor interfaces although in this case we have ignored gravity.[18] It may also describe a coarse-grained interface in a three-dimensional Ising model, but only when above the roughening temperature (since $h_{m,n}\in\mathbb{R}$). The dynamics of the model can be studied using methods analogous to $d=2$, from which one can obtain the moment generating function for the moments of $h_{0,0}$, for an initially flat interface, which is

$$\langle \exp[ih_{0,0}(t)\phi]\rangle = \exp[-\tilde{\alpha}_L(t)\phi^2]\,, \tag{17}$$

where

$$\tilde{\alpha}_L(t)=\sum_{n=0}^{L-1}\sum_{m=0}^{L-1}\frac{1-\exp\left\{-4\sigma\Gamma t\left[2-\cos\left[\frac{(2n+1)\pi}{2L}\right]-\cos\left[\frac{(2m+1)\pi}{2L}\right]\right]\right\}}{4\sigma L^2\left[2-\cos\left[\frac{(2n+1)\pi}{2L}\right]-\cos\left[\frac{(2m+1)\pi}{2L}\right]\right]}. \tag{18}$$

The analysis of $\tilde{\alpha}_L(t)$ proceeds as before, where for an interface of infinite extent we have

$$\lim_{L\to\infty}\tilde{\alpha}_L(t)=\frac{1}{4\sigma}\int_0^{4\sigma\Gamma t}dxe^{-2x}[I_0(x)]^2. \tag{19}$$

By again using the limiting properties of I_0 one obtains

$$\lim_{L\to\infty}\tilde{\alpha}_L(t)\sim\begin{cases}\Gamma t & \text{for } t\to 0,\\ \frac{1}{8\pi\sigma}\ln(4\sigma\Gamma t) & \text{for } t\to\infty,\end{cases} \tag{20}$$

showing a logarithmic growth in the nondiffusive regime.

For the case of a large but finite interface we have that

$$\tilde{\alpha}_L(t)\sim\frac{1}{4\pi\sigma}\ln(2L)-\frac{1}{\sigma}g\left[\frac{\sigma\Gamma t}{L^2}\right] \quad \text{for } L\to\infty,\ t\to\infty, \tag{21}$$

where

$$g(x)=\frac{2}{\pi^2}\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\frac{\exp\{-\frac{1}{2}\pi^2x[(2n+1)^2+(2m+1)^2]\}}{(2n+1)^2+(2m+1)^2}. \tag{22}$$

The limiting behavior of $g(x)$ was determined to be (using the Poisson summation formula for small x)

$$g(x)\sim\begin{cases}-\frac{1}{8\pi}\ln x & \text{for } x\to 0,\\ \frac{1}{\pi^2}\exp(-\pi^2x) & \text{for } x\to\infty.\end{cases} \tag{23}$$

Again, one can see that $g(x)$ for $x\to 0$ coincides exactly with (20) for $t\to\infty$. Hence, just as with $d=2$, we have identified three limiting scaling regimes.

To summarize then, we have been able to derive expressions showing how the interface width of an initially flat interface increases with time. This was done for both two and three dimensions using an unweighted Gaussian model (defined on a lattice) obeying Langevin dynamics. In particular, there are three limiting regimes of diffusive growth, $\langle h_0^2\rangle\propto t$, for $t\to 0$; nondiffusive growth, $\langle h_0^2\rangle\propto t^{1/2}(\propto\ln t)$ when $d=2(=3)$, for $t\to\infty$ with $t/L^2\to 0$; and exponential relaxation to the equilibrium thickness $\langle h_0^2\rangle\propto L(\propto\ln L)$ when $d=2(=3)$, for $t/L^2\to\infty$.

The growth in the region where $t\to\infty$ with $t/L^2\to 0$ can be alternatively understood by an argument due to Villain[19] which goes as follows. One assumes that for large t, an interface of infinite extent contains along it a characteristic length $\xi_\parallel(t)$ which grows according to some power law. Guided by theories describing late stage growth of clusters in systems such as binary alloys,[20] this can be assumed to be $\xi_\parallel\propto t^{1/3}$ when the order parameter is conserved and $\xi_\parallel\propto t^{1/2}$ for unconserved order parameters. One then conjectures that the interface width $w(t)$ scales with $\xi_\parallel(t)$ in the same way that the width of a finite-size interface at equilibrium scales with its side length; that is $w^2(t)\propto\xi_\parallel(t)$ for $d=2$ and $w^2(t)\propto\ln\xi_\parallel(t)$ for $d=3$. Using these arguments one is able to reproduce the correct scaling form in expressions (12) and (20) for $t\to\infty$ [including the prefactors of the logarithm in (20)] if one takes $\xi_\parallel\propto t^{1/2}$ independent of d (unconserved order parameter). That the correlation length $\xi_\parallel(t)$ takes this form has been *confirmed* for our model by evaluating the correlation function $\langle h_0(t)h_j(t)\rangle$ for both two and three dimensions.[11]

The limiting properties derived in this paper are in full agreement with results derived from continuum models attempting to describe surfaces of granular aggregates[2] and random deposition with surface diffusion.[4] Indeed, it is easy to see that Eq. (4) and its three-dimensional analog become *stochastic diffusion* equations when making the continuum approximation. Such equations have been studied[2,4] although with different boundary conditions ($\nabla h=0$ at the ends of the interface instead of $h=0$) and with finite-size effects incorporated by use of an "infrared" mode cutoff. The present approach avoids such an approximation.

The simulations of Family[4] for the two-dimensional random deposition model also give scaling behavior consistent with our $d=2$ results. This might suggest (as implied by Plischke *et al.*[5]) that both thickening to equilibrium of an Ising interface and growth due to random deposition with surface diffusion, fall into the same universality class (which is different to that of the Eden cluster and ballistic deposition; believed to be due to the presence of a nonlinear term in their associated Langevin equations[21]). In any case, it is hoped that the results of this paper, which are by no means restricted to the limiting regimes alone, might act as a guide to, for example, Monte Carlo simulations on Ising models containing interfaces. It has also been suggested[22] that our model could provide some understanding to the kinetics of roughening, although for systems with unconserved order parameters as opposed to the previously studied kinetic roughening models which conserve particle number.[23]

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