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Abstract

A one dimensional model of coarsening is developed in which the domain boundaries are points on a line, either finite (with periodic boundary conditions) or (doubly) infinite, and a domain is an interval between any two adjacent points. The postulated equation of motion for the length l of a given interval depends only on the two nearest neighbor interval lengths, yields a zero average rate of change of interval lengths and makes the state of equal interval lengths unstable. It is proved that coarsening occurs by the disappearance of intervals. A special power law form of the equation of motion, treated by an approximation which ignores correlations of the lengths of neighboring intervals, shows a self–similar behavior with an asymptotic distribution of reduced interval lengths at long times that is time–independent. Comparison of the approximate results with computer simulations is made.

1. Introduction

Coarsening is a process in which the scale of a structure increases with time. In the cases we seek to represent by a simple model, a nearly fixed total volume of material is redistributed over a decreasing number of domains, as smaller domains transfer material to larger domains and ultimately disappear. As a result, the average volume of the remaining domains increases and the configuration of the system coarsens. The domains may completely fill the space of the system (grains in a polycrystal) or may be embedded in a matrix (precipitate coarsening). The process is driven by the reduction of the free energy (or area in the simplest cases) of the interfaces between domains or between the domains and the matrix.

A one dimensional model of coarsening has been introduced by Hunderi, Ryum and Westengen [1] in their discussion of models of grain growth. It consists of a linear array of spherical bubbles with nearest neighbor connections through which incompressible gas flows at a rate proportional to the pressure difference between the adjacent bubbles; as a result, gas flows from smaller to larger bubbles. The equation of motion of the ith bubble is taken to be

$$R_i^2\dot{R}_i = M\left(\frac{1}{R_{i+1}} + \frac{1}{R_{i-1}} - \frac{2}{R_i}\right), \tag{1}$$

where R_i is the radius of the ith bubble, M is a constant and the dot denotes differentiation with respect to time. When a bubble disappears, its former neighbors become nearest neighbors. Since the total volume of bubbles in a finite ring is conserved ($\Sigma_i R_i^2\dot{R}_i = 0$), the result, except for very special initial conditions (e.g. equal bubbles), is that the bubbles coarsen until only one bubble remains containing all the gas. The model is attractive despite its artificiality because it is simple enough to allow some elementary analysis and yet rich enough to display many features of more complex models.

Computer simulations [1,2] of the model based on Eq.(1) yield, after an initial transient and before the number of bubbles becomes too small, a time–independent distribution $Q(\sigma)$ of reduced bubble radii $\sigma = R/\langle R\rangle$, where $\langle R\rangle$ is the average radius. Fig.(1) shows a plot of the results of a simulation carried out by Viñals [2] starting with 10^6 bubbles uniformly distributed over σ from 0 to 2. The coincidence of the two symbols representing two different times shows that $Q(\sigma)$ is substantially independent of time; it is also independent of the initial distribution.

In this paper, we investigate a one dimensional model of coarsening based on a generalization of Eq.(1) in which the domains are intervals on a line rather than bubbles; both a finite number of intervals on a finite line with periodic boundary conditions (i.e. a ring of intervals) and an infinite number of intervals on the doubly infinite line are considered. The model is a nearest neighbor one in the sense that the rule of motion of the point (domain boundary) separating two adjacent intervals depends only on the lengths of these intervals.

A theorem is developed for the model that allows the proof that domains do disappear so that the model does indeed show coarsening; for the infinite case, the proof requires a bound that is established in the appendix. When the equation of motion of the domain boundaries has the special form of the power law discussed in section 8, an approximate treatment of the infinite case that ignores correlations between neighboring interval lengths shows that a time–independent distribution $P(\rho)$ of reduced interval lengths $\rho = l/l_c$ develops asymptotically as $t \to \infty$; here $l_c = \text{const.}\langle l\rangle$ is a critical length, where $\langle l\rangle$ is the average interval length. The treatment is based on a generalization of the coarsening theory of Lifshitz and Slyozov [3] and of Wagner[4]. Both the result of this approximate treatment and the simulation results strongly suggest that the asymptotic time–independent distribution of ρ is a rigorous consequence of the power law equation of motion, but this has not been established.

The development of the distribution $P(\rho)$ is an example of what has been called statistical self–similarity (SSS) [5,6]. An evolving system may be defined to be in a SSS mode if any two consecutive configurations brought to the same scale by uniform magnification are statistically indistinguishable, or, alternatively, if any statistical parameter of the system that is invariant under uniform magnification is also independent of time. Many systems, studied in experiments and in simulations, show time–independent distributions of reduced domain sizes [5–8]. A general theory that would reveal the conditions under which these distributions develop does not yet exist.

2. The nearest neighbor coarsening model

Let the position of the domain boundary points on the line be denoted by x_i and the length of the domains or intervals by $l_i = x_{i+1} - x_i$; when two boundary points meet, they coalesce into one new boundary point and the corresponding interval or domain disappears as shown in Fig.2 in which time is the vertical axis. Suppose, at any given instant, the surviving intervals are labeled consecutively. The equation of motion for a boundary point x_i is then assumed to be a function of the nearest neighbor interval lengths of the form

$$\dot{x}_i = f(l_i) - f(l_{i-1}) , \tag{2}$$

where it is assumed that $f(l)$ is a continuous function of l with a continuous derivative; additional characteristics of the function are specified below. From the definition of l_i , and

Eq.(2) it follows that

$$\dot{l}_i = f(l_{i+1}) + f(l_{i-1}) - 2f(l_i)\,. \tag{3}$$

The linear bubble model is a special case of Eq.(3) with $l=R^3$ and $f(l) = M/3l^{1/3}$.

In this paper, we will consider both an infinite array of intervals on the doubly infinite line, and also a finite "ring" of N intervals in which the first and Nth intervals are nearest neighbors. The finite case is completely equivalent to the infinite case with the periodic boundary conditions $l_{i+N}=l_i$ for $N \geq 2$; when N=1, the infinite case consists of an infinite sequence of equal intervals whereas the finite case may be regarded as consisting of only one distinct domain formed by removing any boundary point resulting from the collapse of a previous second interval. In the rest of this paper, we will suppose that $N \geq 2$ for the finite case.

It is clear that the sum of Eq.(3) over a finite ring of N intervals gives

$$\sum_{i=1}^{N} \dot{l}_i = 0\,. \tag{4}$$

The corresponding result for the infinite case is discussed in section 6.

We define a static solution to be one for which $\dot{l}_i = 0$ for all intervals i. Eq.(3) shows that a sufficient condition for a static solution is that $l_i=a$ for all i. In order for the model to represent coarsening, we require the static solution to be unstable. A perturbed solution

$l_i = a + \epsilon_i$, where $|\epsilon_i| << a$, yields, from Eq.(3),

$$\dot{\epsilon}_n = f'(a)\left(\epsilon_{n+1} + \epsilon_{n-1} - 2\epsilon_n\right) \quad , \tag{5}$$

where the prime denotes the derivative. A solution of Eq.(5) of the form $\epsilon_n =$ $A\exp[\omega_m t - i\frac{2\pi}{M}n]$, where $i = \sqrt{-1}$ and M is the wavelength (for a finite ring of N intervals, M must divide N), gives

$$\omega_m = 2f'(a)[\cos(\frac{2\pi}{M}) - 1] \; . \tag{6}$$

For instability, we require $\omega_m > 0$ for all appropriate M and for all a. Therefore we must have $f'(a) < 0$ for all a, that is, f(l) is assumed to be a strictly monotone decreasing function of l.

3. Special case of alternating interval lengths

A special case that is exactly soluble and that clearly shows coarsening by the disappearance of intervals is that in which the initial length of odd numbered intervals is given by $l_o(0) = \bar{l} + a$, and of even numbered intervals by $l_e(0) = \bar{l} - a$; in the finite case, this requires the total number of intervals to be even. It follows from Eq.(3) and the initial conditions that $l_e(t) + l_o(t) = 2\bar{l}$, where the average $\bar{l}$ is constant, as long as all intervals are still present. This relation may be combined with the Eq.(3) to obtain a formal solution for $l_e(t)$ and $l_o(t)$. The time T required for all even intervals to collapse to zero length is then given by

$$T = \frac{1}{2}\int_{\bar{l}-a}^{0} \frac{dy}{f[2\bar{l}-y]-f[y]} < \frac{1}{2}\,\frac{\bar{l}-a}{f[\bar{l}-a]-f[\bar{l}+a]} \, , \tag{7}$$

where the inequality holds because f(l) is a decreasing function of l. Therefore, for any $a > 0$, the average interval size will have doubled after an elapsed time T.

One can see qualitatively that intervals disappear in the general case because, according to Eq.(3) an interval that is and remains less than either neighbor will continue to decrease until it disappears. Proving the disappearance of intervals by tracking individual intervals seems difficult, however, since the actual intervals of minimum length can change; furthermore, the magnitude of $\dot{l}$ for a given minimum interval can become arbitrarily small if adjacent intervals approach the same value of l as the given interval. For these reasons, we will develop some global theorems in the next sections as a basis for the investigation of the disappearance of intervals.

4. The total variation theorem for the finite ring

Theorem 1: If N is fixed and if not all intervals are equal then the total variation V(t) of the sequence of interval lengths given by

$$V(t) = \sum_{i=1}^{N} |l_{i+1} - l_i|, \tag{8}$$

is an increasing function of t.

Proof: We define consecutive (local) minima π_k and maxima Π_k of the sequence of lengths as follows: a maximum Π_k is the length of an interval that is longer than the first interval encountered in either direction with a length different from Π_k; the subscript k indicates that it is the kth maximum. Similarly, a minimum π_k is the length of an interval that is shorter than the first interval encountered in either direction with a length different from

π_k. It follows from hypothesis that there must be at least one pair of extrema in the sequence. Then taking absolute values into account, we have

$$V(t) = 2\sum_{k=1}^{K}[\Pi_k - \pi_k], \tag{9}$$

where K is the number of maxima (equal to the number of minima). But all maxima are increasing functions of time since each one must be the length of one or several adjacent intervals and Eq.(3) shows that $\dot{l} > 0$ for at least one of these intervals; similarly, all minima are decreasing functions of time. Furthermore, as long as no intervals disappear, extrema cannot be destroyed; they may be created in pairs by an interval overtaking or falling below a neighbor. Therefore we see from Eq.(9) that $V(t)$ is an increasing function of time for constant N as claimed.

5. The G theorem for finite N

Let $g(l)$ be an auxiliary function of l whose integral from 0 to l exists and introduce the abbreviations $f_i = f(l_i)$ and $g_i = g(l_i)$. Then multiplying Eq.(3) by g_i and summing on i we obtain

$$\sum_{i=1}^{N} g_i \dot{l}_i = -H \tag{10}$$

where

$$H = \sum_{i=1}^{N} g_i \left(f_{i+1} + f_{i-1} - 2f_i\right) = \sum_{i=1}^{N} h_{i,i+1} \tag{11}$$

in which

$$h_{i,i+1} \equiv h(l_i, l_{i+1}) = (g_{i+1} - g_i)(f_{i+1} - f_i). \tag{12}$$

Eq.(12) shows that $h_{i,i+1} = h_{i+1,i}$. If g(l), like f(l), is a strictly decreasing function of l, then $h_{i,i+1} \geq 0$ for all i, where the equality holds only if $l_i = l_{i+1}$ for all i; therefore, in this case $H \geq 0$. Similarly, if g(l) is a strictly increasing function of l, then $h_{i,i+1} \leq 0$ for all i where again the equality holds only if $l_i = l_{i+1}$ for all i; therefore, in this case, $H \leq 0$. In either case, if $H = 0$, then $h_{i,i+1} = 0$ for all i, which requires $l_i = a$ for all i. Thus Eq.(10) shows that the static solution discussed in section 2 is unique, that is, $\dot{l}_i = 0$ for all i implies $H = 0$ which implies $l_i = a$ for all i.

We next define

$$G(l) = \int_0^l g(l')dl', \tag{13}$$

and

$$G_T = \sum_{i=1}^{N} G_i \;, \tag{14}$$

where $G_i = G(l_i)$; it follows from Eq.(13) that $\dot{G} = g\dot{l}$. Then since $G(l) \to 0$ as $l \to 0$, we obtain from Eqs.(10)–(14) the following result:

Theorem 2 (the G theorem),

$$dG_T/dt = -H\,. \tag{15}$$

To obtain information about the moments of the distribution of interval lengths, we choose $g(l) = nl^{n-1}$, with $n > 1$ so that $g(l)$ is strictly increasing. Then from Eqs.(13)–(14), $G_T = \Sigma_i l_i^n \equiv M_n$, which is the nth moment of the l_i for integral n, and Eq.(15) shows that

$$dM_n/dt = -H^{(n)} \geq 0, \tag{16}$$

where $H^{(n)}$ is given by Eq.(11) with

$$h^{(n)}_{i,i+1} = h^{(n)}_{i,i+1} = n(l_{i+1}^{n-1} - l_i^{n-1})(f_{i+1} - f_i) \leq 0\,; \tag{17}$$

the superscript n refers to the special form of h for this moment case.

6. Disappearance of intervals for finite initial N

The disappearance of intervals for finite N is governed by the following theorem:

Theorem 3: If the initial state of a finite sequence of N intervals of total length L is not static, then N must decrease.

Proof: Assume that N were to remain fixed. Then it is shown below that $H^{(n)} \leq H_{ub} < 0$, where H_{ub} is a negative upper bound, so that, according to Eq.(16), M_n would increase without bound as $t \to \infty$. But this is impossible since M_n is bounded by L^n. Therefore N must decrease and intervals must disappear.

To obtain the upper bound H_{ub} for $H^{(n)}$, for fixed N and an initial non–static state of variation V_0, we observe that there must be at least one pair of consecutive intervals of length l' and l'' at time t such that $|l' - l''| \geq V/N > V_0/N$, where V is the variation at time t and where the last inequality holds because of theorem 1; otherwise the sum in Eq.(8) could not equal V. Hence we obtain the following inequality:

$$H^{(n)} \leq h^{(n)}(l',l'') \leq \mathrm{MAX}_{l'} h^{(n)}(l',l'+V_0/N) = H_{ub} < 0, \tag{18}$$

where $\mathrm{MAX}_{l'}$ denotes the maximization of the expression that follows over the possible range of values of l', which cannot exceed $0 \leq l' \leq L$. The first inequality in Eq.(18) holds because of Eqs.(11) and (17), the second holds because, for any given $l' < l''$, $h^{(n)}(l',l'')$ is a decreasing function of l'' and the last inequality holds because $V_0 > 0$ and the range of values of l' is limited. The result H_{ub} of the maximization process is evidently independent of time. This completes the proof of theorem 3.

Theorem 3 may be applied repeatedly as intervals disappear, provided that the disappearance of an interval never results in a state in which the remaining intervals are of equal length. The latter may occur for special initial conditions (e.g. from an initial state of three intervals, two of equal length and the third shorter), but it seems clear that the subspace of these initial conditions (interval lengths) for N intervals is of lower dimension than N–1 so that we may conclude that almost all initial conditions for N intervals lead to one final interval or domain.

Since a finite ring of intervals is equivalent to an infinite periodic sequence of intervals, we may conclude that any non–static periodic sequence of intervals will evolve to a sequence of equal intervals, each longer than the original average length.

7. The disappearance of intervals from an infinite sequence

We assume that the infinite sequence of intervals on the doubly infinite line is statistically stationary, at any given time, and can be described by probability density functions. Thus let $P(l,t)$ be the density function for intervals of length l at time t. We also introduce the density function

$$n_L(l,t) = N_L(t)P(l,t) \tag{19}$$

for the number of intervals of length l per unit length of line, where

$$N_L(t) = \int_0^\infty n_L(l,t)dl \tag{20}$$

is the total number of intervals per unit length of line at time t.

Since intervals are not created and are not destroyed when finite, the following continuity equation [5] holds on an abstract l axis:

$$\frac{\partial n_L}{\partial t} + \frac{\partial}{\partial l}\left(<\dot{l}|l> n_L\right) = 0\,, \tag{21}$$

where

$$<\dot{l}|l> = \int_0^\infty \dot{l}\, P(\dot{l}|l)d\dot{l} \tag{22}$$

is the expected value of $\dot{l}$ given l, in which $P(\dot{l}|l)$ is the conditional probability density for $\dot{l}$

given l. Substituting Eq.(19) into Eq.(21), we find

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial l}\left(<\dot{l}\,|\,l> P\right) - (\dot{N}_L/N_L)P \;. \tag{23}$$

Equation (23) may be integrated over l to obtain

$$(\dot{N}_L/N_L) = \lim_{l\to 0} <\dot{l}\,|\,l> P \;, \tag{24}$$

assuming that as $l \to \infty$, $\lim <\dot{l}\,|\,l> P = 0$. Eq.(24) shows that N_L decreases as a result of the flux of intervals into the point l=0 on the l line. From the relation $N_L<l> = 1$, it follows that $(\dot{N}_L/N_L) = -(1/<l>)d<l>/dt$, which shows that the average interval size increases as a result of the disappearance of shrinking intervals.

To prove that intervals must disappear from any initial state that is not static, we will need to study the time dependence of the average value of G (Eq.(13)) given by

$$< G > = \int_0^{\infty} G(l)P(l,t)dl \;. \tag{25}$$

Differentiating Eq.(25) with respect to time, using Eq.(23), integrating by parts and using Eq.(13), we obtain

$$d< G >/dt = < g\dot{l} > \; - (\dot{N}_L/N_L)< G > \;. \tag{26}$$

To obtain an expression for the first term on the right hand side of Eq.(26), we rewrite the rule of motion given by Eq.(3) in the form

$$\dot{l} = f(l_+) + f(l_-) - 2f(l)\,, \tag{27}$$

where l_+ and l_- denote the lengths of the intervals to the right and to the left respectively of the interval of length l. It follows immediately from Eq.(27) that $< \dot{l} > = 0$ which is the analog of Eq.(4) for the finite case. Furthermore, multiplying Eq.(27) by g(l) and averaging, we obtain the analog of Eq.(10), namely,

$$< g(l)\dot{l} > = -\eta, \tag{28}$$

where

$$\eta = < h(l,l_+)>. \tag{29}$$

in which

$$h(l,l_+) = h(l_+,l) = [g(l_+)-g(l)][f(l_+)-f(l)] \tag{30}$$

For a finite ring, comparision of Eqs.(11) and (29) shows that $\eta = H/N$. Combining Eqs.(26) and (28), we have

$$d< G >/dt = -\eta - (\dot{N}_L/N_L)< G > . \tag{31}$$

Theorem 4: If the initial value $\eta(0)=\eta_0$ of $\eta(t)$ is non–zero, then $\dot{N}_L < 0$, that is, intervals must disappear.

Proof: Choose g(l) to be a positive continuous decreasing function of l with a contiuous derivative (e.g. g(l)=exp[–l]) so that $\eta_0>0$. Suppose, contrary to the assertion of theorem, intervals do not disappear so that $\dot{N}_L = 0$ (intervals are not created in the model). Then Eq.(31) shows that $< G >$ would be a decreasing function of time. But it is shown in the appendix that if $\eta_0>0$, and if intervals do not disappear, then $\eta(t) \geq \eta_{lb}$, where $\eta_{lb} > 0$ is a positive time–independent lower bound. Therefore, $< G >$ would become negative in a time not exceeding $< G >_0 / \eta_{lb}$, where $< G >_0$ is the initial value of $< G >$. But this is impossible since g(l) and hence $< G >$ can never be negative (Eqs.(13) and (25)). Therefore intervals must disappear as claimed (i.e. $\dot{N}_L < 0$).

Theorem 4 can be applied at any time at which η does not vanish. Assuming that we can ignore initial conditions that lead to a static solution after the disappearance of a set of intervals, we conclude that the disappearance of intervals continues indefinitely.

8. Treatment of the power law form of f(l) by the mean neighbor approximation

In this section, we investigate the consequences of the particular power law form of f(l) given by

$$f(l) = Al^{\beta}, \quad A\beta < 0\,, \tag{32}$$

where the condition on A and β assures that f(l) is a decreasing function of l; when $\beta = 1/3$, we recover the linear bubble model with $l = R^3$ (Eq.(1)). It will be shown that, in the random order approximation (ROA) described below, the model based on Eq.(32) with $\beta \leq 1$ develops a time–independent distribution $P(\rho)$ of reduced interval lengths $\rho = l/l_c$ in the asymptotic limit $t \to \infty$; here l_c is a critical length that is a constant times the average interval length $<l>$. The ROA assumes that interval lengths are randomly ordered on the line so that correlations of the lengths of neighboring intervals are ignored. The use of this approximation permits the application of a generalization [9] of the classical theory of Lifshitz and Slyozov [3] which establishes the asymptotic time–independent distribution $P(\rho)$.

From the result of the ROA approximation and from the suggestive evidence of the simulations of Eq.(1), it seems very plausible that an asymptotic distribution $P(\rho)$ would follow rigorously from the model based on Eq.(32) (with $\beta \leq 1$), but this has not been shown. It has been conjectured [6] that a necessary condition for the development of a time–independent distribution of reduced interval lengths is that the rule of motion for $\dot{l}$ be such that the ratio of $\dot{l}$ for any two intervals remain invariant under a uniform magnification of the system; Eq.(32) fulfills this condition.

We first develop the ROA approximation. The average of Eq.(27) over all intervals of length l is, rigorously,

$$<\dot{l}\,|l> = <f(l_+)|l> + <f(l_-)|l> - 2f(l). \tag{33}$$

where $< . |l>$ indicates the conditional average for a fixed l. According to the ROA, $<f(l_+)|l> = <f(l_-)|l> = <f(l)>$, so that Eq.(33) becomes, in this approximation,

$$<\dot{l}\,|l> = 2[<f(l)> - f(l)]. \tag{34}$$

It is convenient to define a critical length $l_c(t)$ by the condition

$$f(l_c) = <f(l)>, \tag{35}$$

so that Eq.(34) becomes

$$<\dot{l}\,|l> = 2[f(l_c) - f(l)]; \tag{36}$$

we see that in the ROA approximation, intervals for which $l > l_c$ grow on the average, and intervals for which $l < l_c$ shrink on the average.

Now, using Eq.(32) in Eq.(36) and introducing the variable $\rho = l/l_c$, we obtain

$$l_c^{1-\beta} <\dot{\rho}\,|\rho> = 2A[1-\rho^\beta] - y\rho, \tag{37}$$

where

$$y = l_c^{-\beta}\, \dot{l}_c\,. \tag{38}$$

The null curve for which $<\dot{\rho}\,|\rho> = 0$ in the (ρ,y) phase plane is given, from Eq.(37), by

$$y = \frac{2A[1-\rho^\beta]}{\rho}\,. \tag{39}$$

According to the generalized LSW theory [9], this curve must either have a maximum (ρ_m,y_m) or must increase monotonically to a horizontal asymptote (y_m) in order for a stable time–independent distribution of $P(\rho)$ to develop asymptotically at long times. The condition for this to be true is, from Eq.(39), $\beta \leq 1$. Furthermore, according to the theory, the stable operating point of the system corresponds to $y=y_m$. By differentiation of Eq.(39) we find

$$\rho_m = (1-\beta)^{-1/\beta}, \tag{40}$$

$$y_m = \frac{2A(1-\rho_m^{\beta})}{\rho_m}. \tag{41}$$

For constant $y=y_m$, we integrate Eq.(38) and then make the approximation, appropriate in the asymptotic limit of long times, that $t>>t_0$ and $l_c(t)>>l_c(t_0)$, to obtain

$$l_c^{1-\beta} = (1-\beta)y_m t \quad \text{for } \beta < 1, \tag{42}$$

$$l_c = \text{const.}\exp[y_m t] \quad \text{for } \beta = 1 . \tag{43}$$

Substituting Eq.(42) into Eq.(37) and rearranging, we obtain, for $\beta<1$,

$$<\dot{\rho}|\rho> = \frac{F(\rho)}{t}, \tag{44}$$

where

$$F(\rho) = \frac{2A[1-\rho^{\beta}]-y_m\rho}{(1-\beta)y_m}; \tag{45}$$

for β=1 we obtain, from Eq.(37),

$$<\dot{\rho}\,|\,\rho> = 2A\ , \tag{46}$$

where we have used the relation $y_m = -2A$ for the asymptote obtained from Eq.(39).

Following the general procedure of LS theory, we write the continuity equation for $\tilde{n}_L(\rho,t) = n_L(l,t)(dl/d\rho)$,

$$\frac{\partial \tilde{n}_L}{\partial t} + \frac{\partial}{\partial \rho}\left(<\dot{\rho}\,|\,\rho>\ \tilde{n}_L\right) = 0. \tag{47}$$

The form of $<\dot{\rho}\,|\,\rho>$ given by Eqs.(44) and (46), when used in Eq.(47) allows a general solution $\tilde{n}_L(\rho,t)$ to this equation to be written down. When this general solution is subjected to the condition expressing the conservation of interval length per unit length of line, that is, $N_L<l> = 1$, or

$$l_c\int_0^\infty \tilde{n}_L(\rho,t)\rho d\rho = \int_0^\infty n_L(l,t)ldl = 1, \tag{48}$$

the result is a time–independent probability distribution $P(\rho)$ for ρ that has the following forms:

For the case $\beta < 1$, one finds

$$P(\rho) = \frac{-1}{(1-\beta)F(\rho)} \exp\left[\frac{1}{1-\beta}\phi(\rho)\right], \quad \text{for } 0 \le \rho \le \rho_m, \tag{49}$$

$$P(\rho) = 0\ , \qquad \text{for } \rho > \rho_m\ ,$$

where

$$\phi(\rho) = \int_0^{\rho} \frac{d\rho'}{F(\rho')} . \tag{50}$$

In this case, $P(\rho)$ clearly has a sharp cutoff at ρ_m, since $F(\rho_m)=0$ (Eq.(45)). Other characteristics of $P(\rho)$ have been discussed elsewhere [9].

For the case $\beta=1$, one finds

$$P(\rho) = \exp[-\rho] . \tag{51}$$

The continuous curve of Fig.3 is a plot of Eq.(49) for the case of the linear bubble model based on Eq.(1); the points represent the simulation. The discrepancy is due to the presence of correlations of interval or bubble sizes with relative position that are ignored in the ROA approximation. The correlations favor larger than average bubbles adjacent to smaller than average bubbles.

The LS theory and its generalizations prove the stability of the asymptotic distributions discussed above only with regard to a limited set of perturbations [9] corresponding to constant values of y. It would be desirable to extend these to include arbitrary time dependent perturbatons to be sure that the distributions are indeed stable.

9. Summary and discussion

A one dimensional model of coarsening has been developed in which the domain boundaries are points on a line, finite or (doubly) infinite, and the domains are intervals defined by any two adjacent points. The postulated equation of motion for the length l of an interval depends only on the two nearest neighbor intervals, yields a zero average rate of change of interval length and makes the state of equal interval lengths unstable. If an interval shrinks to zero length, its former neighbors become nearest neighbors.

It is proved that, in general, intervals do disappear, in both the finite and the infinite cases, and hence that the model does exhibit coarsening. A special power law form of the equation of motion for the interval length is investigated with the use of a random order approximation (ROA) which ignores correlations of the lengths of neighboring intervals. The result, obtained by the use of a generalized Lifshitz–Slyozov theory, is an asymptotic distribution of reduced interval lengths at long times that is time–independent. Comparison of the approximate results with computer simulations shows that length correlations are in fact developed by the model, in which larger than average intervals tend to be adjacent to smaller than average intervals and vice versa. Based on the results approximate treatment, and on the computer simulation results, it is speculated that a rigorous treatment of the power law model, including correlations, would also show a (different) time–independent distribution of reduced lengths.

There is considerable evidence [5–8] from experiment, simulations and theory, that coarsening systems develop asymptotic self–similar behavior, as exemplified by the time–independent distribution of reduced interval lengths. This behavior is also shown by a one dimensional stochastic model of coarsening, recently discussed [10], in which the boundary points execute random walk. Asymptotic self–similarity has been discussed in terms of renormalization group theory [11–12]. Very little is known, however, about the general conditions under which self–similarity is to be expected.

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Figure captions

1. The probability distribution $Q(\sigma)$ of reduced radii $\sigma = R/\langle R \rangle$ for the linear bubble model from simulation results: crosses represent twice the simulation time as the diamonds

2. Schematic diagram of coarsening in the one dimensional model with time as the vertical axis.

3. The probability distribution $Q(\sigma)$ of reduced radii σ for the linear bubble model: the curve shows the ROA results and the black dots denote simulation results.

Appendix

We assume that the auxiliary function g(l) used to define η (Eqs.(29)–(30)) is positive, continuous and strictly decreasing with a contiuous derivative. We wish to show that if no intervals disappear and if $\eta(0) > 0$ then $\eta(t) \geq \eta_{lb} > 0$, where η_{lb} is a time–independent lower bound of $\eta(t)$.

Corresponding to the finite case, a stationary sequence of interval lengths, will contain a subsequence whose lengths are (local) extrema consisting of minima (π_k) alternating with maxima (Π_k). Eq.(3) shows that the value of a maximum cannot decrease, although the interval that possesses this value may shift; correspondingly, the value of a minimum cannot increase. As discussed in section 4, extrema may be created in pairs but cannot be destroyed. The subset of minima π_k at any time t that were originally present at t=0 will be denoted by γ_k and the corresponding subset of maxima by Γ_k; actually, we will use density functions to describe the distribution of γ and Γ.

We define a block to be the sequence of consecutive intervals between a given adjacent γ,Γ pair, in either order; if two or more adjacent intervals have the same extremum value, any one of these may be chosen as the block boundary for the present purpose. Then using $d\Omega = d\gamma d\Gamma$ for an element of area in the γ,Γ plane and integrating over the region $\Gamma \geq \gamma \geq 0$, we may write η (Eq.(29)) as

$$\eta = \int b_0(\gamma,\Gamma,t)H_0(\gamma,\Gamma)d\Omega$$

$$+\int\int b_1(\gamma,\Gamma,l,t)H_1(\gamma,\Gamma,l)d\Omega dl$$

$$+\int\int\int b_2(\gamma,\Gamma,l_1,l_2,t)H_2(\gamma,\Gamma,l_1,l_2)d\Omega dl_1 dl_2$$

$$+ \dots \quad , \tag{52}$$

In Eq.(52), the integrations over the l's extend from 0 to ∞, $b_m(\gamma,\Gamma,l_1,l_2, \dots l_m,t)d\Omega dl_1 \dots dl_m$ is the number of blocks per interval with block boundaries γ and Γ, in the range $d\Omega = d\gamma d\Gamma$ containing m intervals in the range $dl_1 \dots dl_m$ at time t, and $H_m(\gamma,\Gamma,l_1,l_2, \dots l_m)$ is given by

$$H_m(\gamma,\Gamma,l_1,l_2, \dots l_m) = h(\gamma,l_1) + h(l_1,l_2) + \dots h(l_m,\Gamma) \tag{53}$$

where the notation is consistent with that of Eq.(11) and where, as before,

$$h(x,y) = [g(x) - g(y)][f(x) - f(y)] \geq 0; \tag{54}$$

the equality holds in Eq.(54) only if x=y.

We proceed to show that, for fixed γ and Γ, there is a set of values $l_i = \bar{l}_i$ that yield a minimum value $\bar{H}_m(\gamma,\Gamma)$ of $H_m(\gamma,\Gamma,l_1,\dots l_m)$ which may therefore be used in Eq.(52) to obtain a time–dependent lower bound $\bar{\eta}(t)$ for η; we further develop the properties of $\bar{H}_m(\gamma,\Gamma)$ necessary to construct the desired time–independent lower bound η_{lb}.

To show that H_m has a minimum value $\tilde{H}_m$, for fixed γ and Γ, we first show that the insertion of an interval of length l between any two intervals of length l_1 and l_2, such that $l_1 < l < l_2$, always decreases H. Thus calling H_0 the value of H for the block with no contained interval and H_1 the value of H for the block containing one interval, we have

$$H_0 - H_1 = h(l_1,l_2) - [h(l_1,l) + h(l,l_2)]$$

$$= [g(l_1)-g(l)][f(l)-f(l_2)]+[f(l_1)-f(l)][g(l)-g(l_2)] > 0, \qquad (55)$$

where we have used Eq.(54) and where the inequality holds since both g and f are decreasing functions of l.

It follows from this result that an upper bound for $H_m(\gamma,\Gamma,l_1,l_2..l_m)$ is $H_0(\gamma,\Gamma)=h(\gamma,\Gamma)$ and that any values of the l's between γ and Γ decrease H_m below the upper bound. Furthermore, for $\Gamma > \gamma$, H_m is strictly positive since there must be at least one positive term in Eq.(53). Therefore, since H_m is continuous and differentiable in the l's, it must attain a minimum value

$$\tilde{H}_m(\gamma,\Gamma) = h(\gamma,\tilde{l}_1) + h(\tilde{l}_1\tilde{l}_2) + \ldots h(\tilde{l}_m,\Gamma) > 0, \qquad (56)$$

for a set of values $l_i=\tilde{l}_i$ that satisfy the set of m equations

$$h_y(l_i,l_{i+1}) + h_x(l_{i+1},l_{i+2}) = 0\,, \quad \text{for } i=0,1,\,..\, m-1 \qquad (57)$$

where $l_0= \gamma$ and $l_{m+1}= \Gamma$, and where the subscripts x and y denote partial derivatives of

$h(x,y)$. Equations (57) cannot be satisfied unless $l_i \leq l_{i+1} \leq l_{i+2}$, so that the solutions $\tilde{l}_i(\gamma,\Gamma,m)$ of Eqs.(57) form a sequence of lengths that increase with i from γ to Γ; here i may increase to the left or the right in the sequence of intervals.

It follows from Eq.(55) that $\tilde{H}_m(\gamma,\Gamma)$ is a decreasing function of m. Thus, Eq.(55) shows that inserting an interval of intermediate size between any two intervals in the minimum sequence of m intervals will lower H and the readjustment of interval sizes required to minimize the resulting m+1 sequence will further lower H so that

$$\tilde{H}_{m+1}(\gamma,\Gamma) < \tilde{H}_m(\gamma,\Gamma) . \tag{58}$$

The additional required properties of the $\tilde{H}_m(\gamma,\Gamma)$ are obtained by differentiating Eq.(56) with respect to γ and Γ, for a given block containing m intervals, to obtain, respectively,

$$\partial\tilde{H}_m(\gamma,\Gamma)/\partial\gamma = h_x(\gamma,\tilde{l}_1) < 0 \quad , \tag{59}$$

$$\partial\tilde{H}_m(\gamma,\Gamma)/\partial\Gamma = h_y(\tilde{l}_m,\Gamma) > 0 \quad , \tag{60}$$

where we have used Eqs.(57) to cancel all implicit derivatives with respect to the $\tilde{l}_i$, regarded as functions of γ and Γ, and where we have used $h_x(x,y) \leq 0$ and $h_y(x,y) \geq 0$ for $y \geq x$, which follow from Eq.(54).

We now establish the lower bound η_{lb} in three stages: First the lower bounds $\tilde{H}_m(\gamma,\Gamma)$ may be substituted for the H's in Eq.(52) and the resulting terms integrated over the l_i's to obtain

$$\eta(t_0) \geq \tilde{\eta}(t_0) = \int \sum_{m=0}^{\infty} B_m(\gamma,\Gamma,t_0)\, \bar{H}_m(\gamma,\Gamma) d\Omega\,, \tag{61}$$

where $B_m(\gamma,\Gamma,t_0)d\Omega$ is the number of blocks per interval with γ and Γ in the range $d\Omega=d\gamma d\Gamma$ containing m intervals at time t_0; it is the result of integrating the corresponding b_m over the l_i's.

Secondly, we wish to establish a lower bound for $\tilde{\eta}(t_0)$ by restoring the original extrema to their original values at t=0, holding fixed the number of intervals in each block. In this comparison system, denoted by a hat, $\hat{B}_m(\gamma,\Gamma,t)d\Omega$ is the number of blocks per interval with γ and Γ in the range $d\Omega = d\gamma d\Gamma$ at time $t \leq t_0$, containing m intervals. Then since each block of fixed m is a conserved entity, the $\hat{B}_m$ satisfy the following continuity equation in the γ,Γ plane:

$$\frac{\partial}{\partial t}(\hat{B}_m) + \frac{\partial}{\partial \gamma}(<\dot{\gamma}>\hat{B}_m) + \frac{\partial}{\partial \Gamma}(<\dot{\Gamma}>\hat{B}_m) = 0\,, \tag{62}$$

where $<\dot{\gamma}>$ and $<\dot{\Gamma}>$ denote the expected values of the rates of change of the extrema (in the actual and comparison system) as a function of γ and Γ. Further, we define $\hat{\eta}(t)$ by the expression

$$\hat{\eta}(t) = \int \sum_{m=0}^{\infty} \hat{B}_m(\gamma,\Gamma,t)\, \bar{H}_m(\gamma,\Gamma) d\Omega\,; \tag{63}$$

we see from Eqs.(61) and (63) that $\hat{\eta}(t_0)=\tilde{\eta}(t_0)$, since the number of contained intervals in each block is the same in the real and comparison sequence at $t=t_0$ and hence $\hat{B}_m(\gamma,\Gamma,t_0) = B_m(\gamma,\Gamma,t_0)$. Differentiating $\hat{\eta}$ in Eq.(63) with respect to time, using Eq.(62), integrating by parts and setting the integrated parts equal to zero since $\hat{H}_m$ vanishes on the boundary $\gamma=\Gamma$ and $<\dot{\gamma}>\hat{B}$ vanishes on the boundary $\gamma=0$ (no intervals disappearing), we obtain

$$d\hat{\eta}(t)/dt = \int \sum_{m=0}^{\infty} \hat{B}_m\Big[<\dot{\gamma}>(\partial\hat{H}_m/\partial\gamma)+<\dot{\Gamma}>(\partial\hat{H}_m/\partial\Gamma)\Big]d\Omega \geq 0, \tag{64}$$

where the inequality follows from the inequalities $<\dot{\gamma}> \leq 0$ and $<\dot{\Gamma}> \geq 0$ combined with Eqs.(59)–(60). Therefore we conclude that

$$\eta(t_0) \geq \tilde{\eta}(t_0) = \hat{\eta}(t_0) \geq \hat{\eta}(0). \tag{65}$$

Thirdly, we note that $\hat{\eta}(0)$ still depends on t_0 because it is based on the number of contained intervals in each block at time t_0. We therefore impose a redistribution of contained intervals so as to minimize $\hat{\eta}(0)$ as defined by Eq.(63). That is, we define a time–independent lower bound η_{lb} as the minimum of Eq.(63), at $t_0=0$, obtained by choosing the functions $\hat{B}$ subject to the constraint

$$\nu = \int \sum_{m=0}^{\infty} m\hat{B}_m(\gamma,\Gamma,0)d\Omega\ , \tag{66}$$

where ν is the number of contained intervals per interval in the actual sequence at t=0, and the constraint

$$\mathcal{B}(\gamma,\Gamma,0) = \sum_{m=0}^{\infty} B_m(\gamma,\Gamma,0) = \sum_{m=0}^{\infty} \hat{B}_m(\gamma,\Gamma,0), \tag{67}$$

where $\mathcal{B}(\gamma,\Gamma,0)$ is the actual number density function for γ and Γ at $t = 0$.
The result is the desired time–independent lower bound since, using Eq.(65) (dropping the subscript), we have $\eta(t) \geq \hat{\eta}(0) \geq \eta_{lb}$; furthermore, η_{lb} cannot vanish, for otherwise Eqs.(63), (67) and the definition of the B's show that, for $t = 0$ and $\gamma \neq \Gamma$, $\hat{B}_m = \hat{B}_m = b_m = 0$ for all m, which in turn would imply $\eta(0) = 0$ (Eq.(52)), contrary to hypothesis.

Further details of the minimization process leading to η_{lb} will not be discussed except to say that it is not difficult to establish that

$$\tilde{H}_{m+2} + \tilde{H}_m - 2\tilde{H}_{m+1} > 0 \, . \tag{68}$$

so that the sum in Eq.(63) may be eliminated in favor of an integrand involving the product $\mathcal{B}(\gamma,\Gamma,0)\tilde{H}_{\bar{m}}$, where $\bar{m}$ is a weighted average value of m. One may then discuss the minimization process in terms of the Lagrangian multiplier technique.

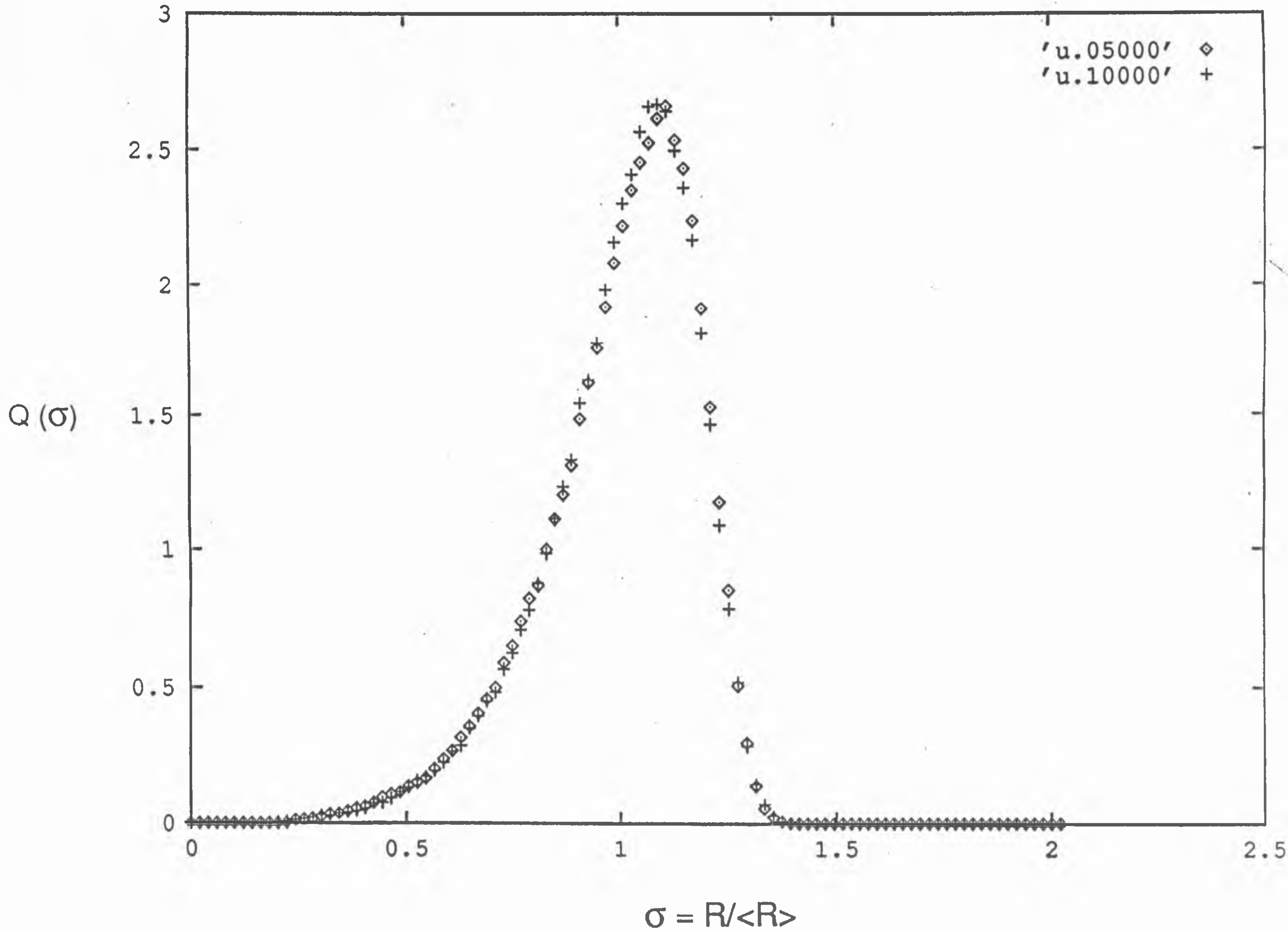

FIG. 1

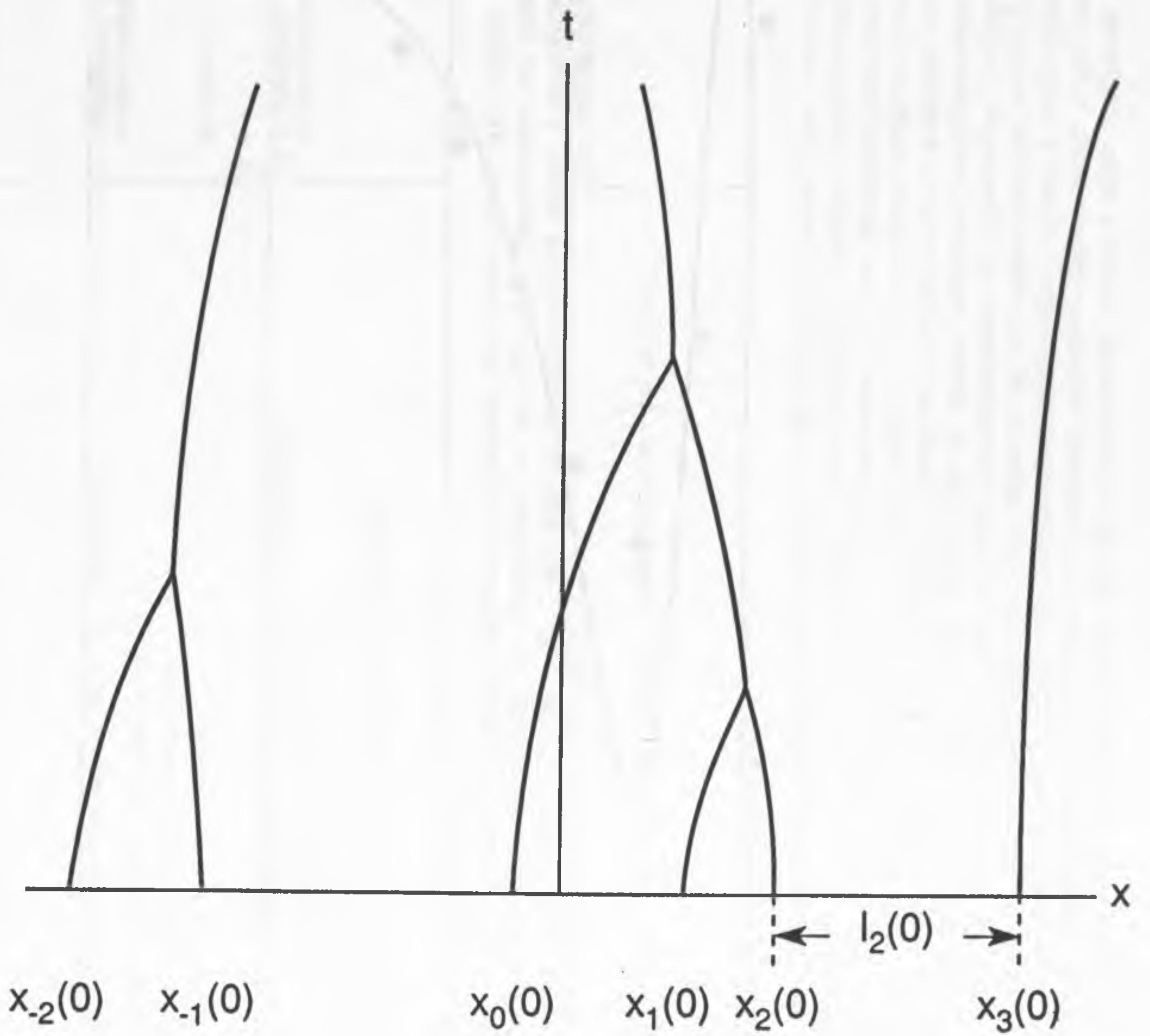

FIG. 2.

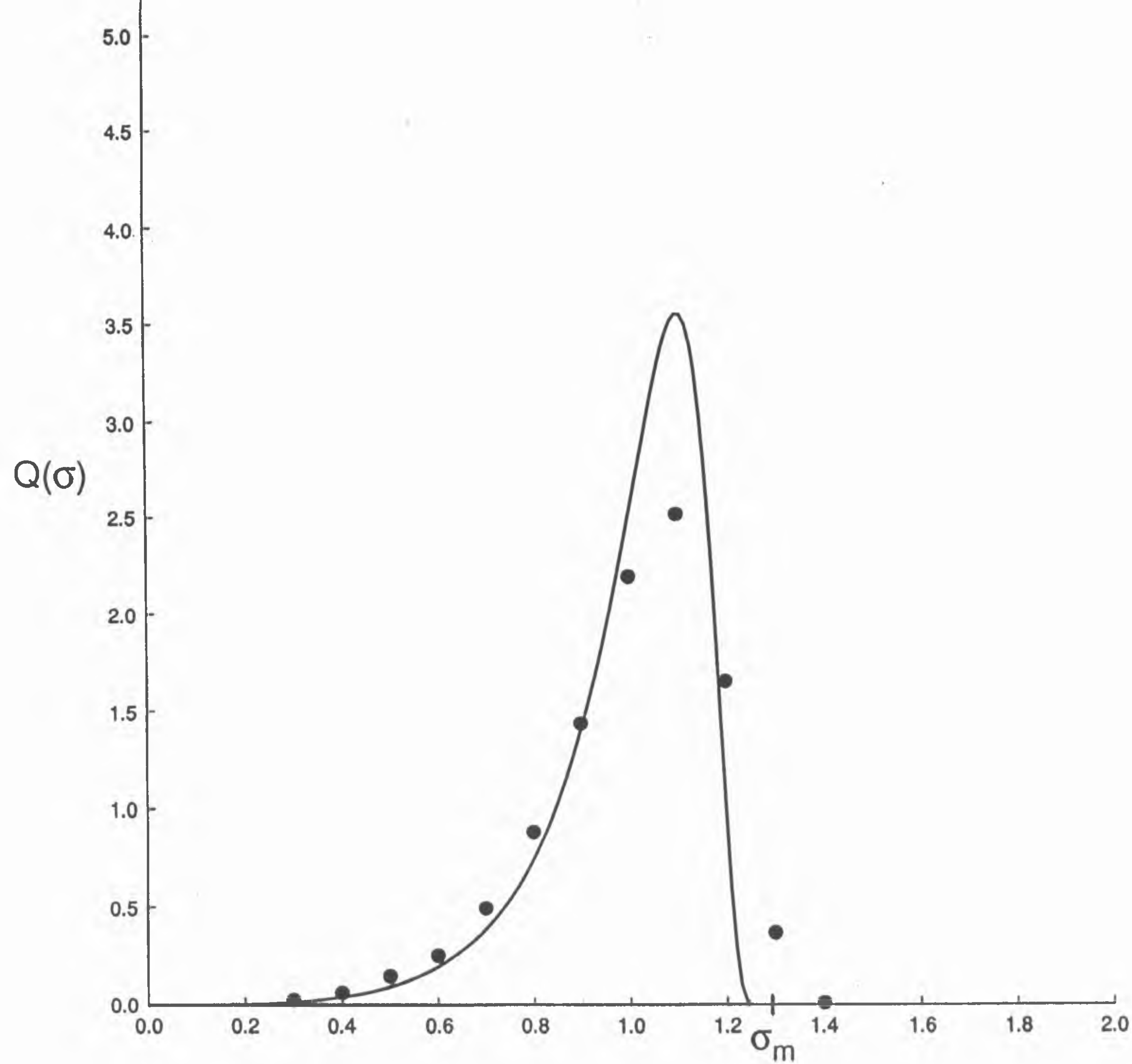

FIG. 3

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13. ABSTRACT *(Maximum 200 words)*

A one dimensional model of coarsening is developed in which the domain boundaries are points on a line, either finite (with periodic boundary conditions) or (doubly) infinite, and a domain is an interval between any two adjacent points. The postulated equation of motion for the length l of a given interval depends only on the two nearest neighbor interval lengths, yields a zero average rate of change of interval lengths and makes the state of equal interval lengths unstable. It is proved that coarsening occurs by the disappearance of intervals. A special power law form of the equation of motion, treated by an appoximation which ignores correlations of the lengths of neighboring intervals, shows a self-similar behavior with an asymptotic distribution of reduced interval lengths at long times that is time-independent. Comparison of the approximate results with computer simulations is made.

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