Scaling behavior in stochastic growth models exhibiting dynamical phase transitions and degenerate spin-glass order in diluted frustrated systems

Ph.D. Thesis by
Hüseyin KAYA, M.Sc.
50994003312

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Supervisor (Chairman): Prof. Dr. Ayşe ERZAN
Members of the Examining Committee Prof. Dr. A. Nihat BERKER (M.I.T.)
Prof. Dr. Hamit YURTSEVEN (İ.T.Ü.)
Prof. Dr. Figen KADIRGAN (İ.T.Ü.)
Assoc. Prof. Dr. Meral AYDIN (H.Ü.)

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DİNAMİK HAL DEĞİŞİMİ İÇEREN STOKASTİK BÜYÜME MODELLERİNDEKİ ÖLÇEKLENME DAVRANİŞI VE SEYRETLİMLİS BUNALIMLI SİSTEMLERDEKİ DEJENERE SPİN-CAMI DÜZEĞİ

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DOKTORA TEZİ
Y. Müh. Hüseyin KAYA
509940033012

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Tezin Savunulduğu Tarih : 19 Temmuz 1999

Tez Danışmanı : Prof.Dr. Ayşe ERZAN  
Diğer Jüri Üyeleri  
  Prof.Dr. A. Nihat BERKER (M.I.T.) 
  Prof.Dr. Hamit YURTSEVEN (İ.T.Ü.) 
  Prof.Dr. Figen KADIRGAN (İ.T.Ü.) 
  Doç.Dr. Meral AYDIN (H.Ü.)

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DINAMİK HAL DEĞİŞİMİ İÇEREN STOKASTİK BÜYÜME MODELLERİNDEKİ ÖLÇEKLENME DAVRANIŞI VE SEYRELİTMİŞ BUNALIMLI SİSTEMLERDEKİ DEJENERE SPIN–CAMİ DÜZENİ

ÖZET

Bu tez çalışmasında, dengede ve dinamik hal değişimleri içeren üç farklı fiziksel sistem incelenmiştir. Bunlar, yönelimli (directed) sızmalar (percolation), yüzeylenme–tepkime (adsorption–reaction) arayüzey modeli ve seyreltilmiş üçgen örgüde antiferromanyetik Ising modelidir.

Tavlımsız karışıklık (annealed disorder) içeren ve dinamik hal değişimi gösteren en basit sistemlerden birisi yönelimli sızmadır. İzotropik olmayan ölçekenme davranış gösteren bu modelin kritik üstelleri hala kesin olarak elde edilememiştir. Biz, iki boyutta yönelimli sızmının kritik üstellerini hesaplayabilmek için dinamik kabalastırma (coarse–graining) içeren ve sabit ölçük dönüşümü (fixed–scale transformation) dan yararlanan bir gerçekçuez renormalizasyon grubu yaklaşma gelişirdik. Hesaplanan kritik üsteller bilinen en iyi sonuçlarla uyum göstermektedir.


SCALING BEHAVIOR IN STOCHASTIC GROWTH MODELS EXHIBITING DYNAMICAL PHASE TRANSITIONS AND DEGENERATE SPIN–GLASS ORDER IN DILUTED FRUSTRATED SYSTEMS

SUMMARY

In this thesis, three different kinds of systems which exhibit equilibrium and dynamical phase transitions were investigated. These are directed percolation, an adsorption–reaction interface model, and the antiferromagnetic Ising model on a dilated triangular lattice.

Directed percolation is one of the simplest systems containing annealed disorder and exhibiting a dynamical phase transition. The critical exponents of this model which obeys anisotropic scaling behavior are not known exactly. In order to calculate the critical exponents, we develop a novel position–space renormalization–group approach based on a dynamical coarse-graining procedure and the fixed–scale transformation. The exponents we found are in good agreement with well-known results.

The other model which exhibits dynamical phase transitions contains only adsorption and reaction processes, with annealed disorder due to random deposition of particles. As the average interface velocity is taken to zero, the self–affine interface with Kardar–Parisi–Zhang like scaling behavior undergoes a delocalization transition with new critical exponents that fall into a novel universality class. As the critical point is approached, the interface becomes a multi–valued, multiply connected self–similar set. The scaling behavior and critical exponents are determined from Monte Carlo simulations and scaling arguments.

In the other study, we consider the antiferromagnetic Ising model on triangular lattice, in equilibrium. By using the hard–spin mean–field theory developed by Netz and Berker, the phase transitions of the fully frustrated system are investigated under the quenched dilution of spins belonging to one of the three sublattices. Our results show that since random spin dilution relieves the frustration at random localities, after a threshold dilution, the system exhibits uniform and opposite magnetization in the undiluted sublattices. Furthermore, the spin–glass order parameter also departs from zero in all the sublattices. Our most important result is that within the ordered phase, multiple sets of solutions which show no ultrametricity are obtained.
1. INTRODUCTION

Phase transitions and critical phenomena have been a central issue of statistical physics for many years. In particular, both equilibrium and dynamical phase transitions with or without external noise have attracted special interest.

One key notion which emerged through these studies is the notion of universality. According to the universality hypothesis, a variety of continuous (or second-order) phase transitions can be classified into a small number of universality classes determined by a few basic properties characterizing the system under study, such as the space dimensionality $d$, the symmetry of the order parameter, and the range of interaction. The scaling behavior, i.e., the critical exponents, are uniform throughout a universality class.

In recent years, it has been observed that disorder also has a very important role in the understanding of phase transitions, because the symmetry of the systems can usually be broken down due not only to the extreme values of control parameters and external fields, but also due to disorder.

Disorder may be quenched or annealed. Quenched disorder, which has typical relaxation times many orders of magnitude larger than those of the dynamical variables, and may be considered spatially fixed and independent of time, usually corresponds to impurities or defects in materials. On the other hand, annealed disorder is associated with degrees of freedom whose typical turnover times are comparable to those of the dynamical variables of interest, or emerges in the stochastic nature of the dynamics such as random deposition of particles on a growth surface, etc..

Directed percolation, which has emerged as one of the generic dynamical systems with absorbing states obeys self-affine scaling properties, is the simplest example of a dynamical phase transition driven by annealed noise. The absorbing
state where all paths terminate is a trap from which the system cannot escape, the dynamics does not go on indefinitely. The tunable parameter $p$ is the occupation probability of a site or a bond or, in other words, the propagation probability. For $p \gtrsim p_c$, where $p_c$ is the threshold value, activity persists as time tends to infinity, and the connected paths in the spatio–temporal domain form an infinitely large cluster, i.e., the percolating cluster. This can be compared with the equilibrium phase transition of static percolation. On the other hand, the edge of the directed percolation can be thought of as a moving interface or a growth model. In chapter 2, a novel position–space renormalization–group scheme will be described with dynamical coarse–graining for bond–directed percolation in two dimensions. Its critical exponents and threshold value for the bond occupation probability will be calculated.

In chapter 3, we will propose an adsorption–reaction interface model driven by annealed randomness, and investigate its dynamical scaling behavior with different assumptions. It will be shown that this adsorption–reaction interface model exhibits self–organized critical behavior, with self–affine scaling properties. The scaling behavior undergoes a crossover from one universality class to another, near a critical point that is reached by tuning the degree of randomness in the system. At this critical point we have a delocalization of the interface, that is, the divergence of the width of the interface with time. Concurrently, a phase transition takes place between anisotropic and isotropic behavior, as the growth direction becomes completely delocalized.

In chapter 4, the fully frustrated antiferromagnetic triangular Ising model with random quenched site dilution will be studied. This is a case where order is enhanced due to the (quenched) randomness introduced by randomness. It is of interest to study the effect of dilution on the phase diagram, the existence of spin–glass order, and the multiplicity of ordered phases by using the closed–form implementation of hard–spin mean–field theory, since it is expected that this dilution will randomly remove some of the frustration, giving rise to order at finite temperatures. Overlaps (or, similarity) and distances (or, dissimilarity) between pairs of solutions will be discussed.
2. POSITION–SPACE RENORMALIZATION GROUP FOR
BOND DIRECTED PERCOLATION IN TWO DIMENSIONS

Directed percolation has been studied extensively [1-6], since it plays very
important role in a large variety of non-equilibrium systems with a single absorbing state [7]. A wide array of dynamic processes as fluid flow through a porous medium in an external field [8], forest fires [9,10] or epidemic growth models [11], reaction-diffusion systems [12-14], damage spreading [15], self-organized criticality [16], models of growing surfaces with roughening transition [17-19], etc. fall into the same universality class as directed percolation. There is no exact result for the critical exponents characterizing the dynamical phase transition separating the absorbing steady state from the active phase. The correlation length exponents in the longitudinal and transverse directions, defined via $\xi_\parallel \sim |p - p_c|^{-\nu_\parallel}$ and $\xi_\perp \sim |p - p_c|^{-\nu_\perp}$, and the percolation threshold $p_c$ have been found to great accuracy by series expansion methods [5,6] to be $\nu_\parallel = 1.733$, $\nu_\perp = 1.097$ and $p_c = 0.6447$, respectively.

The fixed-scale transformation (FST) [20] introduced by Pietronero, Erzan, and Evertsz [21,22] has been used to investigate the self-similar properties of irreversible growth models, namely, diffusion–limited aggregation [23] and dielectric breakdown [24], as well as other intrinsically critical growth problems such as cluster-cluster aggregation [25]. The FST has also been applied to systems such as percolation [26], Ising or Potts models [27], invasion percolation [28,29] and to directed percolation [30] at the critical point. Renormalization group ideas have been used in conjunction with the FST approach [31], in order to identify the scale invariant growth rules in terms of which the finite cell fixed–scale transformation matrix should be computed, with good results. Forest fires [32] (which fall into the same universality class as directed percolation) and the sandpile model [33,34] have been studied by means of the “dynamically driven renormalization group” [35], which combines real–space renormalization group ideas with a dynamical steady–state condition reminiscent of the fixed–scale transformation approach.
In this chapter, we would like to introduce a novel position-space
renormalization-group (PSRG) treatment of the directed percolation problem
[36]. This approach modifies conventional PSRG methods in two ways: i) the
weights of different initial states in the RG cell are computed from the steady
state distribution found from the fixed point of the FST; ii) a “dynamical” coarse
graining procedure is defined which allows for the appearance of two different scale
factors in the longitudinal (time-like) and transverse (space-like) directions, thus
taking into account the self-affine nature of the problem. These scale factors are
determined independently, without having to make any additional assumptions.

The chapter is organized as follows. In the next section, we construct the
renormalization–group transformation subject to the dynamical fixed–point con-
dition, and compute the critical parameter as well as the transverse and lon-
gitudinal correlation–length exponents. In the last section we provide a short
discussion.

2.1. RG TRANSFORMATION WITH DYNAMICAL COARSE
GRAINING

We consider 1-time and 1-space dimensional bond directed percolation as a
growth process. Let us recall the growth rules: if a site at time $t$ is active, its two
neighbors at time $t + 1$ may be activated, each independently, with a probability
$p$. If $p$ is larger than the threshold value $p_c$, there is a finite probability that the
growth process is continued indefinitely.

We now outline a renormalization–group procedure which takes into account
fluctuations in regions larger than the renormalization–group cell by using a
steady-state distribution of initial conditions, obtained from the FST. It also
introduces self-consistently determined rescaling lengths, rather than preset scale
factors between the original and coarse grained lattices.

Our renormalization–group cell is shown in Fig.2.1(a). The boxes $AA'BB'$ and
$CC'A'A''$ will coarse grain, under a dynamic coarse graining procedure we describe
below, to the bonds $ab$ and $ac$, as shown in Fig.2.1(b). This process conserves the
transverse and longitudinal directions, but does not conserve the lattice angles,
since these two directions are scaled differently. Rescaling by the appropriate
longitudinal and transverse scale factors will restore the original lattice (Fig.
2.1(c)). The lattice spacing is taken to be $\sqrt{2}$ for convenience, yielding $\ell_L = 1$
and $\ell_\parallel = 1$ for the transverse and perpendicular distances between the nearest
neighbors, such as $AA'$ and $BB'$. Clearly, we only have to consider one of the boxes, e.g., $AA'BB'$ for our renormalization procedure, by symmetry.

![Diagram](image)

**Figure 2.1** The dynamical coarse-graining procedure. (a) The RG cells $AA'BB'$ and $CC'A'A''$ (the bold lines) in the original lattice are coarse-grained (b) to the bonds $ab$ and $ac$ respectively, which are rescaled in the next step (c) to preserve the lattice angles.

To obtain the renormalization transformation for the bond occupation probability $p$, we compute the total probability $P(p)$ that a spanning path exists across the box $AA'BB'$, by considering all the different initial configurations (states of $A$ and $A'$) and the spanning configurations that can be obtained from them. A spanning configuration is defined as one where a path starts from either $A$, or $A'$ or both, and ends on $B$ or $B'$ or both.

### 2.1.1. Steady–State Distribution of Initial Conditions

Since there are two possible origins which can be active both together or by themselves, four different initial configurations have to be considered as illustrated in Fig.2.2. Any spanning configuration may have more than one path which connects the origins to the end points. For instance, two different paths are possible for connecting the sites $A$ and $B'$ in the spanning configuration shown in Fig.2.3.
Figure 2.2 Four different initial configurations are represented. In computing their respective weights, (see text) the bold lines in each configuration are replaced with the probability $p$, and the dashed lines with $1 - p$.

In order to compute the probabilities of finding each initial configuration, say $W_i$, $i = 1, \ldots, 4$, we make use of the time-invariant probabilities for the relative frequency of doubly or singly occupied boxes in a box covering of the equal-time transverse subsets on the cluster of active sites, in terms of the probabilities $p$.

Figure 2.3 Two different paths belonging to the same spanning configuration.

In recent work [30], the FST approach has been used to calculate the fractal dimension of directed percolation at the critical point, given the threshold value of $p$. The main idea underlying the FST approach here is that at the critical point, as $t \to \infty$, the infinite transverse subsets of active sites at any given $t$ are statistically
similar under translation in $t$. In particular, they can be modeled by Generalized Cantor Sets generated by a random sequence of fragmentations obeying a one-parameter, scale-invariant distribution as shown in Fig.2.4. Given a hierarchical partitioning of the transverse subsets into cells of size $2^{-k}$, the relative probability of encountering a singly occupied or doubly occupied cell among nonempty cells at a fixed arbitrary scale is equal to $C$ or $1 - C$. This probability can be computed [30] from the fixed point of the fixed-scale transformation as:

$$C = \frac{2 - 3p + 5p^2 - \sqrt{36 - 108p + 109p^2 - 30p^4 + 9p^4}}{2p^2 + 4p - 4},$$

up to first order in the FST approach.

![Diagram](image)

**Figure 2.4** The generator for the random Cantor set corresponding to a transverse subset of the incipient infinite cluster. Cells of type 1 and type 2 participate in the fine graining process with corresponding probabilities $C_1$ and $C_2$. We represent the activated sites with black circle and inactive sites with white circle.

We now make use of this FST results to compute the normalized weights $W_i$ of the initial configurations $i$ in terms of $C$ and $p$,

$$W_1 = pC/2$$
$$W_2 = (1 - p)C/2 + (1 - p)^2(1 - C)$$
$$W_3 = p(1 - C/2)$$
$$W_4 = p(1 - p)(1 - C).$$

In the following subsection we proceed to obtain the renormalization transformation in terms of which the critical value of $p$ can be determined.

### 2.1.2 The Renormalization Transformation for $p$

Depending on the initial configurations $i = 1, ..., 4$, the total number of possible spanning configurations will be different. One sees that in Fig.2.2 (1) only one;
(2) seven; and (3) – (4) eighteen spanning configurations each are possible. It
should also be noticed that some spanning configurations can be observed in more
than one different initial configuration. For example, the spanning configuration
which contains only one path which starts from \( A' \) and ends at \( B' \) can be observed
in all the initial configurations except the second one (see Fig.2.2). The total
probability \( f_i \) of the spanning cluster for the \( i \)'th initial configuration is given by

\[
\begin{align*}
  f_1(p) &= p^2 \\
  f_2(p) &= p^2 + p^3 - p^4 \\
  f_3(p) &= 2p^2 + p^3 - 3p^4 + p^5 \\
  f_4(p) &= f_3(p)
\end{align*}
\]

The renormalization–group transformation for \( p \) is then found to be

\[
P(p) = W_1 f_1(p) + W_2 f_2(p) + W_3 f_3(p) + W_4 f_4(p) = p'.
\]  \hspace{1cm} (2.1)

The fixed point of this transformation gives the threshold value, \( p_c = 0.6443 \)
which is in agreement up to the third digit with the series expansion \([5,6]\) result,
namely 0.6447.

2.1.3. The Affine Transformation in the Longitudinal and Transverse
Directions

The system has two independent correlation lengths \( \xi_\parallel \) and \( \xi_\perp \), parallel and
perpendicular to the time direction respectively, which diverge with different exponents
as \( \xi_\parallel \sim |p - p_c|^{-\nu_\parallel} \) and \( \xi_\perp \sim |p - p_c|^{-\nu_\perp} \). To compute these exponents,
we use the eigenvalue equations,

\[
\frac{dp'}{dp} \big|_{p=p_c} = b_\parallel^{1/\nu_\parallel}, \quad \frac{dp'}{dp} \big|_{p=p_c} = b_\perp^{1/\nu_\perp}.
\]  \hspace{1cm} (2.2)

We determine the appropriate rescaling lengths \( b_\parallel \) and \( b_\perp \) from,

\[
b_\parallel = \frac{< L_\parallel >}{l_\parallel}, \quad b_\perp = \frac{< L_\perp >}{l_\perp},
\]  \hspace{1cm} (2.3)

in terms of the average projected lengths, \( < L_\parallel > \) and \( < L_\perp > \), of the spanning
paths onto the time and transverse directions as shown in Fig.2.5. These quantities
are the amounts by which the coarse grained lattice (see Fig.2.1(b)) has been
dilated in the “dynamical coarse-graining” step. Since we have taken the lattice
constant to be \( \sqrt{2} \), the projections of a single bond on the original lattice onto
the time and space directions are \( \ell_\perp = \ell_\parallel = 1 \).
Figure 2.5 All possible paths and their extremal projections contributing to the dynamical rescaling factors $<L_\parallel>$ and $<L_\perp>$. See Fig 2.1.

In the time direction, one has to take into account the fact that under coarse graining, different time steps collapse onto each other; that is why we consider each path originating from $A$ or $A'$ and terminating on $B$ or $B'$ as contributing separately to $L_\parallel$. While enumerating the possible paths over which the average is taken, it makes a difference if there is a bond between $A$ and $A'$, since the paths change in case $A'$ is activated by $A$. The same thing holds for the end sites $B$ and $B'$. Note that the result of taking the extremal projections first and then averaging is different from finding the “average path” and then taking its projections. This point will be further discussed below.

For $X \equiv \{\perp, ||\}$, we have

$$<L_X> = \sum_i W_i \sum_\beta q_{i,\beta} \sum_\alpha L_X^{i,\beta,\alpha}, \quad (2.4)$$

where $q_{i,\beta}$ is the relative probability of any spanning path $\beta$ belonging to an initial state $i$, and is to be found from $f_i$ by giving equal weights to the distinct paths in any spanning configuration equally. Substituting the value of $p_c$ found from Eq. (2.1) into Eqs. (2.3,2.4), we find,

$$<L_\perp> = 1.7996$$

and
\[ < L_\parallel > = 2.5561. \]

These values yield, together with Eq.(2.2), the correlation-length exponents to be \( \nu_{\parallel} = 1.719 \) and \( \nu_\perp = 1.076 \), which are comparable with the best known results \([5,6]\) \( \nu_{\parallel} = 1.733 \) and \( \nu_\perp = 1.097 \).

2.2. DISCUSSION

There have been some earlier studies of directed (therefore self-affine) systems via position-space renormalization group (PSRG) techniques. The introduction of two different scaling factors \( b_\parallel \) and \( b_\perp \) due to existence of two independent scaling directions was firstly suggested by Dhar and Phani \([37]\), where they employed a decimation transformation. However, their results are far from the accepted values of the critical exponents and dependent upon their choice of the RG cell, which determines \( b_\parallel / b_\perp \). Very large-cell PSGR calculations by Zhang and Yang \([38]\) are able to accurately reproduce the self-affine behavior of directed self-avoiding walks, but are more appropriately in a class with Monte Carlo. A bond-moving and decimation transformation for anisotropic directed bond percolation in arbitrary dimension \([39]\) and its generalization for other directed systems \([40]\) by da Silva and Droz give the critical fugacity very accurately in all dimensions for directed self-avoiding-walks. For two-dimensional directed percolation, it yields good results for the threshold value \( p_c \) and \( \nu_\parallel \), but is not as good for \( \nu_\perp \). The approach in these papers is in fact very close to ours; however, the way the projections of paths are taken to compute the scaling factors in the two different directions are different.

One may consider two different ways of projecting a path. The approach of da Silva and Droz \([39,40]\) is to draw a vector between the origin and the end point, and take its two components to be the projections of the path. Our is to take the projection to be the transverse or longitudinal distance between the extremal points of the path, as shown in Fig.2.5.

We believe that our method yields a result which corresponds more closely to what is meant by the size of the transverse and longitudinal fluctuations, in that it measures more accurately the actual size of the region over which a coherent flow takes place. This becomes more evident if we consider the incipient infinite cluster of our system for \( p \sim p_c \). In this cluster, there can be many paths which connect some point at time \( t_0 \) to an end point at \( t_0 + t \). Even though the total
number of bonds in these different paths are the same, the spatial size of the
spanned regions can be radically different (see Fig.2.6). Since the transverse
(longitudinal) correlation length corresponds to the spatial (time-like) size of
the fluctuations, it is more appropriate to take the average over the extremal
transverse (longitudinal) extent of each path.

![Diagram](image)

**Figure.2.6** Macroscopic paths with identical end-to-end vectors, but strongly differing extremal projections.

In conclusion, by incorporating the FST fixed-point condition in the deter-
mination of our distribution of initial configurations, and by a new, dynamical
coarse graining procedure which makes use of averages over extremal projections
of spanning paths, we have succeeded in computing the percolation threshold and
the correlation function exponents much more accurately than before.
3. DYNAMICAL SCALING BEHAVIOR OF ADSORPTION–REACTION INTERFACE MODEL

Interfaces which usually occur as a boundary between two phases, or as edges of growing surfaces have been of considerable interest in the last decade. In many systems containing unrelated physical or chemical processes, roughening phenomena may be observed as a common feature. For example, experiments of fire propagation on paper or in a forest, crystal growth, chemical corrosion, electrochemical deposition, growth of bacterial colonies, heterogeneous catalysis, etc., show that each system above produces a kinetically roughened edge (i.e., interface) [41]. Moreover, the kinetics of roughened interfaces have deep connections with the fields as diverse as self-organized criticality, spin-glasses and complex pattern formation [41-44]. Many kinds of idealized stochastic interface growth models were inspired by the experiments above. These models can be listed as the Eden model and its different variants, the Edwards-Wilkinson (EW) model, the Kardar-Parisi-Zhang (KPZ) model, ballistic deposition, pinned interfaces with quenched noise, restricted solid-on-solid (RSOS) models, random deposition with surface diffusion, etc..

Our main motivation is to try to understand geometrical complexity and scaling properties of the roughened interfaces. The first question should be what is the meaning of “roughening phenomena” or “roughening transition”? It can be easily explained by considering, for instance, solid surfaces. As is well known, the microscopic shapes of crystals are often anisotropic and reflect the underlying symmetry of the crystal lattice. When this happens, it implies that the interfacial fluctuations are insufficient to overcome the anisotropy and one observes sharp facets. However, one might imagine that at sufficiently high temperature (but still below melting temperature), the thermal fluctuations of the interface may overcome the anisotropy and the crystal no longer shows sharp facets. The temperature at which this happens is known as the roughening transition temperature. More generally depending on the value of the control parameters which drives the dynamics, such as temperature, rate of deposition or diffusion, etc., the geometry of the interface may become highly convoluted, resulting in an increase
of the width of interface or interfacial region which contains not only the single interface, but also clusters formed during the interface evolution.

The next questions will be, of course, what are their physical properties, and how to predict them? In previous works, it has been observed that the interface configurations contain very large fluctuations which are reminiscent of the critical fluctuations in equilibrium systems. For this reason, it is very natural to think that these interfaces can be characterized [41-44] by means of critical exponents, i.e., by the scaling dimensions of various macroscopic quantities, namely, i.e., the width of the interface, correlation lengths, structure factor, etc. Indeed, characterization of a self-affine interface by a height \( h \) appropriate to a \( d \)-dimensional substrate \( L \), and of the width of the interface \( w(t, L) \) at a time \( t \) by

\[
w(t, L) = \sqrt{(h - \bar{h})^2},
\]

where the bar denotes an average, yields a dynamical scaling law [45],

\[
w(t, L) \sim L^x f \left( \frac{t}{L^z} \right), \tag{3.1}
\]

where the function \( f(x) \to \text{constant for } x \to \infty \) and \( f(x) \sim x^\beta \), with \( \beta = \chi/z \) as \( x \to 0 \). It should be noticed that if the interface configuration does not contain vacancies or overhangs, the average height \( \bar{h} \) and the time \( t \) are identical. The physical meaning of Eq.(3.1) is that the interface roughness for a given value of \( L \) initially grows with time, as

\[
w \sim t^\beta,
\]

in the transient regime where \( \beta \) is called the “early time” exponent. But, eventually, a crossover takes place, and the width of the interface is saturated to a sample-dependent value, due to finite-size effects, that scales as

\[
w \sim L^x,
\]

where, therefore, \( x \) is as called the “roughness” exponent. The so-called “dynamical” exponent \( z \) specifies the scaling of the characteristic time scale which might be taken to be the relaxation time of the steady-state fluctuations as

\[
t \sim L^z.
\]
The exponents $\beta$, $\chi$, and $z$ determine to which universality class the given model belongs.

In the rest of this chapter, the KPZ and EW models which are the mathematical models described by the continuum partial differential equations will be explained with more detail, and, additionally, a very brief explanation of the Eden model and the main observation of the other discrete numerical models will be given.

The Edwards–Wilkinson (EW) model (or, EW equation) [46] is introduced to extract dynamic scaling properties of kinetically roughened surfaces. Edwards and Wilkinson have considered particle sedimentation within a liquid with competing effects of gravitational relaxation, which tends to smooth the surface, and stochastic noise (the settling particles) which tend to roughen it. Under these assumptions, they derived a continuum partial differential equation as

$$\frac{\partial h(\vec{x}, t)}{\partial t} = \nu \nabla^2 h(\vec{x}, t) + \eta(\vec{x}, t),$$

where $h(\vec{x}, t)$ is the surface position, $\vec{x}$ represents the spatial coordinate along the substrate, $\eta$ the space- and time-dependent stochastic noise. The noise is assumed spatially and temporally uncorrelated and gaussian, with

$$\langle \eta(\vec{x}, t)\eta(\vec{x}', t') \rangle = 2D \delta(\vec{x}' - x) \delta(t' - t).$$

Since the EW equation does not contain any non-linear term, it can be solved exactly in $d = 1 + 1$ dimensions by using a Fourier transform, and gives $\chi_{\text{EW}} = 3 - d/2$ and $z_{\text{EW}} = 2$. The EW equation does not contain the effect of the uniform motion, that is, the relative surface fluctuations became independent of the average velocity of translation.

On the other hand, the Kardar–Parisi–Zhang (KPZ) equation [47] (i.e., the “noise-driven Burgers’ equation”) is an improvement of the EW model. These authors have realized that the average translation affects the surface fluctuations significantly and that the effective global forward translation is only the result of the locally normal propagation. They have included in the equation of motion, Eq.(3.1), the simplest non-linear term (i.e., “lateral” component), which is proportional to $\sqrt{1 + (\nabla h)^2}$. This term can be expanded as $1 + 1/2(\nabla h)^2 + \ldots$ by assuming $(\nabla h)^2$ small. That higher order terms can be neglected amounts to not allowing overhangs, and the constant term can be dropped. Thus, the KPZ equation will be written as
\[
\frac{\partial h(\vec{x}, t)}{\partial t} = \nu \nabla^2 h(\vec{x}, t) + \lambda (\nabla h(\vec{x}, t))^2 + \eta(\vec{x}, t).
\]

The critical exponents of the KPZ model are found as \(\chi_{KPZ} = 1/2\), \(\gamma_{KPZ} = 1/3\) and \(z_{KPZ} = 3/2\) by a renormalization–group analysis. This set of critical exponents characterizes a wide range of anisotropic growth phenomena with annealed noise [41], and where the local velocity of the interface increases with the slope. In the limit that the velocity goes to zero or is independent of the slope [43], one gets the EW model. As a consequence, the existence and absence of the nonlinear term \((\nabla h)^2\) gives two different dynamic scaling behavior, i.e., two different universality classes.

In both models, the interface growth is restricted to being single valued, i.e., a multi-valued interface containing overhangs or disconnected parts consisting of clusters is not allowed. In fact, this is not the case for many real systems, because the surfaces are highly convoluted, display large fluctuations, and even the question of how to characterize them is still largely open [50].

The discrete models whose aim to simulate the cluster growth mechanism on computer are governed by dynamical local rules or processes. Perhaps the simplest growth model was introduced by Eden [48] to simulate the growth of tumors. In addition to its biological applications, this model has relevance to many other types of stochastic growth phenomena. When growing an Eden cluster, one of the empty sites next to the perimeter sites is chosen randomly, and it is added to the cluster. A large cluster is obtained after repeating this procedure many times. The exponents obtained from the Eden model are the same as those of the KPZ model, thus falling into same universality class. Experience from the discrete models tells us that the dynamical scaling behavior does not directly depend on many of the microscopic details, if some basic features such as symmetry and locality are respected. Most models of interface motion break spatial isotropy by imposing a preferred growth direction and many require the height of the interface along this direction to be single valued [41,46,47]. It has been shown that these restrictions can produce qualitative changes in the interface morphology [49,50]. For example, they rule out self-similar fractal growth. The role of the annealed and quenched disorder has been studied [19] for the equilibrium and non-equilibrium cases.

In the following sections of this chapter, an adsorption–reaction interface model which exhibits an anisotropic to isotropic phase transition with novel scaling behavior at the delocalization critical point will be given [51].

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3.1. ADSORPTION–REACTION INTERFACE MODEL

As is well known from solid-state physics, it is difficult to get perfect surfaces, because the periodicity of the surface atoms is spoiled as one approaches the surface. In other words, one gets atomic-scale defects such as kinks, steps, adatoms, vacancies, etc. There is abundant evidence that physical and chemical processes at surfaces are strongly influenced by many surface defects, since the defect regions are energetically more favorable for the adsorption, diffusion, desorption, and reaction processes, and therefore play an important role in surface catalysis [52,53].

More precisely, the desorption activation energy of the atoms which land in the defective regions is much higher than the others due to their coordinations with the neighboring sites, that is, coordinatively unsaturated sites. In general, these regions will be traps for adsorbed atoms. These atoms, in turn, may be the nuclei for the cluster (island) growth at increasing the coverage of the adsorbate, or may be desorbed due to unsaturated chemical bonds. As a consequence, the surfaces with defects are highly active catalytically.

Different kinds of adsorption reaction models with or without diffusion and desorption processes are studied very widely in order to investigate their phase transitions, scaling behavior, and clustering properties [54-57]. Reaction fronts formed by the monomer–monomer type reaction,

\[ A + B \rightarrow \emptyset, \]

in heterogeneous systems where the reaction takes place on a two-dimensional substrate [12] are often confined to a narrow "reaction zone" especially if the reactants are either initially segregated or became segregated due to reaction kinetics.

Our present model is motivated by recent findings [52,53] of high reaction rates and strong bonding at surface defects like steps and vacancies in studies of heterogeneous catalysis.

We consider a two-dimensional idealized surface with only one step, terminating a terrace made up of \( A \) particles (Fig.3.1). The surface is exposed to two kinds of incoming particles, namely \( A \) and \( B \), which are allowed to adsorb at first contact, and only on sites adjacent to the step, which we will call "interface sites". The adsorption of \( A \) particles makes the interface advance. The
adsorbing $B$ particles, on the other hand, immediately react with an randomly chosen $A$ neighbor to form a product which leaves the surface. This eats into the step, making the interface recede. We investigate the effect of changing the rate of injection [58] of the two reactants. We do not allow any reactions to take place with the substrate atoms, all of whose neighboring sites are occupied. We assume, for simplicity, that the temperature is low enough so that no surface restructuring occurs: the bonding to the interface sites is sufficiently strong [59] for diffusion along the interface to be prohibited. The kinetics is therefore driven by the adsorption and reaction steps and not by the transport of the reactants.

![Diagram](image)

**Figure 3.1** A Terrace of $A$ particles, with the interface sites, indicated by bullets, neighboring the step.

The interface is initially a perfectly straight line in the $x$ direction that spans the width $L$ of the system, and is located at $h = 0$. Periodic boundary conditions are applied along the $x$ direction and the system height is not restricted. The system is weakly driven so that at any instant only one particle of either $A$ or $B$ type, with probabilities $p_A$ or $p_B = 1 - p_A$, impinges on the interface.

The interface advances or recedes with an average velocity proportional to $\epsilon \equiv p_A - 0.5$. As the system evolves, the surface roughens, and becomes multiply connected, shedding “island” and “lakes” in its wake. The total number of active sites fluctuates in time. In any given adsorption or reaction step, it can increase, decrease, or remain the same depending on the local configuration of the chosen active site. For example, let us consider that an $A$ particle lands on an interface site (see Figure 3.2). i) If the site $\alpha$ is chosen, the new active site will be the site $x$ over it, and the number of active sites remains unchanged, ii) if the site $\beta$ is chosen, there will be no new active site, i.e., there is a reduction in the number of active sites, iii) if the site $\gamma$ is chosen, there will be three new active sites, i.e., the number of active sites will increase by two.
Figure 3.2. An Intersection of the Interface.

The convolutions of the singly connected interface lead to the formation of lakes and islands. The existence of overhangs plays very a crucial role, for the formation of disconnected parts. The adsorption process may create "lakes" in the bulk by closing up the gulf, while the reaction process may cause the formation of "islands" by disconnecting overhangs. Note that the empty sites neighboring $A$ particles lining enclosures within the bulk and those surrounding the islands are also considered interface sites. This really makes the time evolution of the lakes and islands interesting: i) Since they are the disconnected part of the interfacial region, they can be merged with the singly connected interface, which spans the system in the transverse direction from one side to other, under the rules of the dynamics explained above. In this case, a lake or island will disappear within a lifetime short in comparison to its size. ii) Lakes can be filled by $A$ particles via adsorption, and islands can be eaten away by $B$ particles. iii) They can combine with each other, resulting in larger lakes or islands. At $\epsilon = 0$, for finite $L$, this combination process may give rise to spanning strips of $A$–sites after sufficiently long times, i.e., to the existence of more than one spanning string. (This phenomenon is similar to the formation of Liesegang bands [60]).

It is possible to relate the size of overhangs with the island or lake’s sizes. For instance, when the value of $|\epsilon|$ is close to 0.5, only a few lakes or islands with small sizes are created. Correspondingly, there are only a few overhangs with small sizes on the singly connected part. As $|\epsilon| \to 0$, the singly connected interface becomes more decorated, and yields more overhangs with different sizes, so that the rate of the formation of lakes and islands of all different sizes is increased. As a result, the growth direction becomes completely delocalized, and the interface breaks up into an isotropic fractal (see Figure 3.3). In this limit, the thickness of the
interface and the saturation time diverge so that the width of interfacial region keeps on growing indefinitely.

We have performed Monte Carlo simulations for the system sizes of $L = 64, 128, 256, 512, 1024$. It should be noticed that, in our model, there is no slope conservations, or restrictions for overhangs and no quenched disorder. The only disorder is due to random deposition of particles to the interface, which is “annealed disorder”.

Clearly, the geometry of the interface is identical to that of the line of separation between two pure phases of the two dimensional Ising model as has already been studied by Galavotti [61]. However, in the present non-equilibrium system no Gibbs distribution is available and the statistics of the fluctuations have to be determined purely from the dynamics. Observe that the $|\epsilon| \to 0$ limit is analogous to $T \to T_c$, where the surface tension vanishes, and one gets a scale-invariant distribution of interface fluctuations. To give the interface a nonzero velocity, one must introduce an external field.

![Figure 3.3](image.png)

**Figure 3.3.** The interface at $\epsilon = 0$, for early and later stages of growth. The configurations for early time resemble the surface at larger values of $\epsilon$. 
3.2. CHARACTERIZATION OF THE INTERFACE

The fact that our interface is typically multivalued and displays a wealth of different formations gives rise to many questions to be answered. Does the inclusion or exclusion of the disconnected parts change the scaling properties? What is the role of the overhangs? etc. In the following subsections, the interfacial region will be characterized with different assumptions and their dynamical scaling behaviors will be investigated.

3.2.1. Multi-Valued Interface

Now, we want to characterize the multivalued interface, both with disconnected parts included and excluded. We define the width function as

\[ w(l)^2 = \frac{1}{N(l)} \sum_{i}^{N(l)} (h_i - \bar{h}(l))^2 \]  

(3.2)

where \( N(l) \) is the total number of interfacial sites, \( h_i \) the vertical position of the \( i \)th interfacial site and \( \bar{h}(l) \) the mean position of the interface within an interval of size \( l \). The distance \( l \) is defined along \( x \) direction on the substrate as illustrated in Fig.3.4.

![Diagram](image)

**Figure.3.4** The representation of the interval \( l \).

It is found that initially \( w \) grows with time as \( t^{\theta^{kpz}} \). After the transient regime, the width scales with \( l \) as \( w(l) \sim l^{\chi_{eff}} \) for \( l \ll L \). The value of \( \chi_{eff} \) changes with \( p_A \) in such a way that it goes continuously to zero as one approaches \( p_A = 0.5 \), or \( |\epsilon| \to 0 \), as shown in Figs.3.5 and 3.6.
Figure 3.5. The \( l \) dependence of the multivalued width function \( \langle w(l) \rangle \) for a) \( \epsilon > 0 \) and b) \( \epsilon < 0 \).

As it can be seen from Fig.3.6, \( \chi_{\text{eff}} \) has two different values in the limits of \( p_A = 0 \) and \( p_A = 1 \), if the disconnected parts are not excluded. The reasons for this difference can be explained by reference to the short–range characteristics of the dynamics: For \( p_A = 0 \), interface sites are exposed only to \( B \) particles. The adsorbed \( B \) particle definitely reacts with a randomly chosen neighboring \( A \), then they leave the surface. Since each interface site has equal probability to be selected for adsorption, \( A \) particles in an overhang or projection, which have a greater number of neighboring interface sites, have a greater chance to react and to be eaten away. This prevents the interface from being multivalued and convoluted and results in a smoother interface. On the other hand, a few islands with small sizes which can not affect the statistics are still produced although rarely. Indeed, the dynamics is equivalent to Eden growth where \( \chi = 1/2 \), as we have found.

For \( p_A = 1 \), the situation is a little bit different. The only possible process is adsorption. Now tips and overhangs, which have a larger number of interface sites, are favored for growth. In this limit, the formation of overhangs and lakes with small sizes is very common, that is, the interface is more decorated. The total number of interface sites is much more than the case of \( p_A = 0 \). Since the lakes are located very close to the singly connected part, the change in the average height and the term \( \sum (h - \bar{h})^2 \) in Eq.(3.2) will not be very great. But, the increase in the normalizing factor \( N(l) \) will be more. For small distances, this does not alter the value of \( \langle w(l) \rangle \), due to only a few additional interface sites.
But, as $l$ becomes larger, the increase in the width $w(l)$ will not be as fast as expected for $p_A = 0$, due to the normalizing factor. Consequently, the existence of the disconnected parts affects the effective exponent.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3_6.png}
\caption{The effective roughness exponent $\chi_{\text{eff}}$, for disconnected parts of the interface included in (\textcircled{○}) and excluded from (\textbullet) the analysis; $L \leq 1024$. The error bars are comparable to the size of the symbols.}
\end{figure}

Overhangs, lakes, and islands can be eliminated under one-step coarse graining of the surface in the limits of $p_A = 0$ and 1. The exclusion of the disconnected parts yields the same effective exponent $\chi_{\text{eff}} = 1/2$ in both limits as can be seen from Fig.3.5. The characteristic length or size of overhangs and, therefore, the disconnected parts are functions of $\epsilon$. As we decrease $|\epsilon|$, the size of overhangs is increased. When a big island is created by the corrosion of an isthmus, it may affect the orientation of the singly connected interface even globally, by increasing the fluctuations. The same thing may hold by connecting a big island with the singly connected interface, via the adsorption of an $A$ particle, etc. As a result, even though our model has a short range interaction mechanism, these interactions may create global effects, which involves large fluctuations, depending on how near we are to $\epsilon = 0$.

In the presence of overhangs, lakes, and islands, a competing length scale emerges in the system, the “thickness” of the interface, which we can measure by the variance of the height,
\[ y(i) = \left( \frac{1}{n_i} \sum_{j=1}^{n_i} (h_{ij} - \bar{h}_i)^2 \right)^{1/2} \]

with \( n_i \) being the number of interfacial sites above the point \( i \) along the horizontal axis. This “thickness” \( y \) obeys a skewed-Gaussian distribution as is shown in Fig.3.7.

\[ \text{Figure 3.7 The distribution of interface thickness, } P_y(y). \]

The average \( y_L \equiv < y >_L \) has a transient regime, that is, it grows with time for all values of \( \epsilon \) as

\[ y_L \sim t^{\tilde{\beta}} \]

where \( \tilde{\beta} \) is equal to 1/2, and it is a new critical exponent. After the transient regime, it reaches a stable value and then fluctuates around it (see Fig.3.8).

The average value \( y_L \) and the second moment of this distribution both diverge as \( |\epsilon| \to 0 \) with a second new critical exponent \( \nu = 0.55 \pm 0.05 \approx 1/2 \), as

\[ y_L \sim |\epsilon|^{-\nu}. \]

It is found that \( y_L \) obeys the scaling form

\[ y_L \sim t^{\tilde{\beta}} G(|\epsilon|^{-\nu}/t^{1/\zeta}) \]
where $G(v) \sim v$ for $v < 1$ while for $v > 1$, $G(v) \sim \text{const.}$. This also yields a scaling relation for the dynamical exponent of the longitudinal length scale, namely, $\zeta \equiv 1/\hat{\beta}$.

**Figure 3.8** The average $y_L$ versus $t$ is shown for a) $\epsilon = 0.001$, b) $\epsilon = 0.5$.

**Figure 3.9** The divergence of $y_L$ with respect to $\epsilon$ is shown.
Normalizing $w(l)$ in Eq.(3.2) by $y_L$ yields a collapse of the data for all $\epsilon$ as can be seen from Figure 3.11, from which we conclude that

$$w(l) \sim y_L \begin{cases} l^{1/2}/y_L & l^{1/2} \gg y_L \\ \text{const.} & l^{1/2} \ll y_L \end{cases}$$

We see that $\chi_{eff}$ is depressed to zero as the self-affine excursions of the interface are blurred by the thickness of the interface as $y_L$ becomes greater than $l^{1/2}$.

Figure 3.10 The width normalized by $y_L^{1.1}$ crosses over to Eden behavior as a function of $l^{1/2}/y_L$, where $y_L$ is the average variance of the height above any point. The different sections of the curve correspond to data taken at $\epsilon = 0.001, 0.003, 0.005, 0.01, 0.05, 0.1, 0.2, 0.3, 0.4, 0.5$. The deviations from the smooth collapse are due to $l$ becoming comparable to the system size $L = 1024$.

We believe that the exponent of $y_L$ normalizing $w$ will converge to 1 as one takes longer runs and reaches a greater degree of saturation for small values of $\epsilon$.

The thickness of just the singly connected part, which is taken as the distance between the maximum and minimum height, $W$, does not diverge as we near the critical point so that the disconnected parts make up almost all of the interfacial region at the delocalization transition. In the critical region, $W$ grows in time by a power of $1/3$. But, for $\epsilon \gg 0$, the growing process is slower, namely, the power is equal to $1/4$. Note that $W$ keeps growing much after $y_L$, but eventually saturates. In the steady state, the thickness $W$ scales with $l$ as

$$W(l) \sim \begin{cases} l^{1/2} & \text{Eden} \\ l^{2/3} & \text{Isotropic} \end{cases}$$
Figure 3.11 The time dependence of $W(t)$ is represented for $\epsilon = 0.5, 0.001$.

3.2.2. Single-Valued Projections of the Interface

It has previously been pointed out [49] that the presence of overhangs may cause the small-scale structure of an interface to crossover from being self-affine to self-similar, while the large scale behavior is self-affine. To test this hypothesis we first investigate two different ways of defining single-valued profiles of the interface. The first consists of simply taking the average height at any given point, $\bar{h}_i$, i.e.,

$$w_s(l)^2 = \left\langle \frac{1}{l} \sum_i (\bar{h}_i - \bar{h}(l))^2 \right\rangle,$$

while the second, the maximum height for $\epsilon > 0$ (minimum height for $\epsilon < 0$),

$$w_{\text{ext}}(l)^2 = \left\langle \frac{1}{l} \sum_i (h_i^{\text{ext}} - \bar{h}^{\text{ext}}(l))^2 \right\rangle.$$

These width functions exhibit KPZ like scaling with $l$ for all values of $\epsilon$ (see Fig.3.12), as long as $l$ is sufficiently smaller than $L$ both for the case where we include the disconnected parts into our definition of the interface, and for the case where we take only the singly connected spanning string.
3.2.3. Correlation Lengths and Crossover from Anisotropic to Isotropic Behavior

We define longitudinal and transverse correlation lengths, $C_x(l_{ch})$ and $C_h(l_{ch})$, in a symmetrical way particularly suited to revealing the isotropic nature of the interfacial region for length scales smaller than the interface thickness,

$$C_x(l_{ch}) = \langle (x(r + l_{ch}) - x(r))^2 \rangle^{1/2},$$
$$C_h(l_{ch}) = \langle (h(r + l_{ch}) - h(r))^2 \rangle^{1/2}.$$

Here both $r$ and $l_{ch}$ are the ("chemical") length measured along a single spanning string in the interface; $x$ and $h$ are the horizontal and vertical coordinates of the interface site labelled by the chemical distance along the string (see Fig3.13).

The data collapse for $C_h$ and $C_x$ are displayed in Figs.3.14 and 3.15. We find that for small times, $l_{ch} \gg t^{1/2}$ and for $y_L \ll l_{ch}^{1/2}$, i.e., in the Eden limit,

$$C_x \sim l_{ch} \ (y_L \ll l^{1/2}),$$

whereas, for $y_L \gg l_{ch}^{1/2}$
$C_x \sim l_{ch}/t^{\nu} \quad (y_L \gg l_{ch}^{1/2})$.

with $\nu = 1/6$, the horizontal projection decreasing with $t$ as the surface evolves in the critical ($|\epsilon| \to 0$) region. The new exponent $\nu$ is another exponent characterizing the delocalization critical point. On the other hand, for $l_{ch} \ll t^{1/2}$, i.e., in the steady state,

$$C_x \sim \begin{cases} 
  l_{ch} & (y_L \ll l_{ch}^{1/2}) \\
  l_{ch}^{2/3} & (y_L \gg l_{ch}^{1/2})
\end{cases}$$  \hspace{1cm} (3.3)

The longitudinal correlation function grows like

$$C_h \sim t^{1/3}$$

for early times for all values of $|\epsilon|$, while in the steady state ($l \ll t^{1/2}$),

$$C_h \sim \begin{cases} 
  l_{ch}^{1/2} & \text{Eden} \quad (y_L \ll l_{ch}^{1/2}) \\
  l_{ch}^{2/3} & \text{isotropic} \quad (y_L \gg l_{ch}^{1/2})
\end{cases}$$  \hspace{1cm} (3.4)

Figure 3.13 The representation of the chemical distance $l_{ch}$. 

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Figure 3.14 a) $C_h$ and $C_x$ for $\epsilon = 0.5$ for $l_{ch} = 2, ..., L/2$, and different times. b) $C_h$ in the isotropic region, $\epsilon = 10^{-4}$

We see that near the delocalization critical point at $\epsilon = 0$, in the steady state, the interfacial region becomes isotropic, with $C_z \sim C_h$. This region is characterized by an "isotropic" roughness exponent $\chi_{isot} = 2/3$. We summarize the scaling behavior once more in terms of extended homogeneity relations, with $u = l_{ch}/t^{1/z_{KPZ}}$ and $s = y_L/l_{ch}^{KPZ}$, as

$$C_h \sim \alpha_h(\epsilon) \, t^{\gamma_{KPZ}} \, f(u, s)$$
$$C_x \sim \alpha_x(\epsilon) \, t^{1/z_{KPZ}} \, g(u, s)$$

where

$$f(u, s) \sim \begin{cases} \text{const.} & u \gg 1 \\ u \chi_{KPZ} & u \ll 1, \, s \ll 1 \\ u s^{1/z_{KPZ}} & u \ll 1, \, s \gg 1 \end{cases}$$

and

$$g(u, s) \sim \begin{cases} u & s \ll 1 \\ u \chi_{KPZ}/s & u \gg 1, \, s \gg 1 \\ s^{-1/\beta_{KPZ}} & u \ll 1, \, s \gg 1 \end{cases}$$
The amplitudes are defined as $\alpha_x(\epsilon) = (\alpha + |\epsilon|^{1/6})$ and $\alpha_h = 1/(\alpha^{-1} + |\epsilon|^{1/6})$, where $\alpha$ is some constant.

**Figure.3.15** The vertical projection $C_h$ of sections of the singly connected part, plotted as a function of the horizontal projection $C_x$.

From these scaling forms we see that the new critical exponents obey the relationships,

$$\psi = \tilde{\beta} - \frac{1}{z_{KPZ}} + \frac{\chi_{KPZ}}{z_{KPZ}}$$

and

$$\chi_{\text{isot}} = \zeta \chi_{KPZ} / z_{KPZ}$$

which yields,

$$\chi_{\text{isot}} = \beta_{KPZ} / \tilde{\beta} .$$

We may actually find the value of $\chi_{\text{isot}}$ from the following argument. From Eq.s.(3.3,3.4) we see that $l_{ch} \sim C_h^{1/\chi_{\text{isot}}} \sim C_x^{1/\chi_{\text{isot}}}$, and thus the graph dimension of a single strand of the interface is $D_g = 1/\chi_{\text{isot}}$. Since the graph dimension is related to the roughness exponent $\chi$ via $D_g = 2 - \chi$, setting $\chi = 1/2$ yields $\chi_{\text{isot}} = 2/3$. We thus also find, correctly, that $\tilde{\beta} = 1/2$. 

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As the interface crosses over from being self-affine to self-similar within a band of width $y_L \sim |\epsilon|^{-\nu}$, one may compute the fractal dimension of the set of all sites on the multiply connected interface. We use the box counting method in order to calculate the fractal dimension of the interfacial region. In this method, the structure is divided into the boxes whose sizes change with a constant scaling factor, and then the occupied boxes are counted. The slope obtained from the plot of the total number of occupied boxes, $N_k$, via the length scale, $l_k$, in log-log scale gives the fractal dimension such that

$$N_k \sim l_k^{-D_f},$$

where the subscript $k$ describes the level of iteration. The fractal dimension $D_f$ is found to be equal to $1.85 \pm 0.05$ for length scales $l < y_L$, as shown Fig.3.16.

![Figure 3.16](image)

**Figure 3.16** The fractal dimension $D_f$ obtained via the box counting method for the system size $L = 1024$.

At the delocalization point, $\epsilon = 0$, there is a diversity of lakes and islands. The size distribution of islands (or, similarly, lakes) gives a power law dependence such that

$$n_s \sim s^{-\tau},$$

where $\tau = 1.6 \pm 0.1$ (see Fig.3.17).
Figure 3.17 The size distribution of lakes and islands at $\epsilon = 0$.

Additionally, their size distributions obeys

$$P(s) \sim \exp(-s/s_c)/s^\gamma,$$

with $s_c \sim |\epsilon|^{-\gamma}$, where we find $\gamma \simeq 0.9$, and $s_c$ is the size cut-off for the lakes and islands.

Figure 3.18 The size distribution of the disconnected parts at the delocalization critical point, $\epsilon = 0$, converges to $P(s > \sigma) \sim \sigma^{-\gamma+1}$ for late times.

Since we do not expect that there should be yet another length scale present in the problem besides $y_L$, we must have $\gamma = 2\nu$, assuming the islands to have a scaling dimension $D = 2$ (defined by $s \sim l^D$). This is born out numerically to within our error bars. The distribution of the perimeters is likewise a power law.
\[ n_p(p) \sim p^{-\omega}. \]

with the exponent \( \omega = 1.8 \pm 0.1 \). The power law dependence of size distribution and perimeter distribution may yield a scaling relation between the size \( s \) and perimeter \( p \) as

\[ p \sim s^\phi. \]

The exponent \( \phi \) can be calculated by solving the equation below

\[ n_p(p) = \int n(s)\delta(s^\phi - p)ds, \]

which gives

\[ \phi = \frac{\tau - 1}{(\omega - 1)} \approx 3/4. \]

Since the perimeters must scale with the linear size \( l \) of the islands as \( l^{D_\nu} \), \( D \) must be given by \( D = D_\nu/\phi = 2 \), and the islands are indeed compact.

**Figure 3.19** The perimeter area distribution of lakes and islands at \( \epsilon = 0 \).

In conclusion, we have presented an adsorption-reaction model where the interface undergoes a delocalization transition at the point where the mean velocity of the interface goes to zero. Although it has previously been observed [49,50], that the presence of overhangs, islands, and lakes causes the small-scale structure of the interface to crossover from being self-affine to self-similar while the large
scale behavior remains self-affine, we have identified a critical point where the thickness of the interface diverges with a new critical exponent $\nu$, which controls this crossover. Near this critical point, the interface is characterized by new set of critical exponents $\chi_{\text{iso}}$, $\tilde{\beta}$, $\zeta$, $\psi$, and the fractal dimension $D_f$. We relate the critical exponents $\chi_{\text{iso}}$, $\tilde{\beta}$, and $\zeta$ to the KPZ exponents via scaling relations.
4. MULTIPLICITY OF ORDERED PHASES IN FRUSTRATED SYSTEMS OBTAINED FROM HARD-SPIN MEAN-FIELD THEORY

The phase transition of magnets or of 'spin systems' have attracted special interest. Thanks to extensive theoretical and experimental studies, we have now a rather good understanding of the nature of phase transitions of standard ferromagnets and antiferromagnets. By the term 'standard', I mean regular and unfrustrated magnets without randomness and frustration. One of the main features of the magnetic systems with randomness and frustration is spin-glass behaviour. The randomness can be involved to the system by random distribution of the interactions $\pm J$, quenched site or bond dilution, etc..

It is accepted that spin-glasses require two essential ingredients. These are randomness and frustration. Randomness refers to quenched disorder in the interactions between the spins. The spin-glass phase is an example of spontaneous cooperative freezing (or order) of the spin orientations in the presence of the constrained disorder of the interactions. It is thus "order in the presence of disorder".

Frustration refers to conflicts between interactions, or other spin-ordering forces, such that not all can be obeyed simultaneously. The relevance of frustration is that it leads to degeneracy and multiplicity of compromises: for example if one has a set of Ising spins at the corners of a polygon with nearest neighbor interactions randomly $\pm J$, then one cannot satisfy all the bonds if an odd number of them is antiferromagnetic, and the ground state is degenerate. In extensive systems frustration can have major consequences on cooperative ordering.

A "rugged free-energy landscape" is often mentioned as a distinctive characteristic in the discussions of spin-glass systems [62]. One character of the problem is that phase space has a complicated landscape of valleys with many stable or at least metastable equilibrium states, causing long relaxation times and the presence of hysteresis cycles, etc.. Barriers between valleys grow as the temperature is reduced, so that eventually the system behaves nonergodically, being trapped
in a single valley for the duration of experiment. The simplest approximation, namely, mean-field theory, yields that spin-glass ordering is nonunique meaning that there exist a large number of degenerate thermodynamic states with the same macroscopic properties but with different microscopic configurations[62]. However, mean-field theory corresponds to an artificial infinitely connected system and does not respect frustration. Moreover, ultrametricity (i.e., a certain topography of the landscape, or of the multiple solutions) and reentrance phenomena have special interest in spin-glasses.

In this chapter, while applying the hard-spin mean-field theory to the antiferromagnetic Ising model on the triangular lattice which is fully frustrated, it is of interest to investigate the effect of random quenched site dilution on the phase diagram in the absence of external magnetic field. Additionally, the existence of a multiplicity of ordered phases and, if this is the case, their ultrametricity will be investigated [63].

4.1. THE FULLY FRUSTRATED ISING MODEL AND HARD-SPIN MEAN-FIELD THEORY

The antiferromagnetic Ising model on the triangular lattice, with Hamiltonian

\[ -\beta H = -J \sum_{<ij>} s_i s_j, \quad J \geq 0, \]  

(4.1)

where \( s_i = \pm 1 \) at each site \( i \) of a triangular lattice and \( <ij> \) indicates summation over nearest-neighbor pairs of sites, is fully frustrated [64]: In each elementary triangle, one of the three nearest-neighbor antiferromagnetic interactions is dissatisfied when the energy is minimized. This leads, macroscopically, to a highly degenerate system that is disordered at all non-zero \((1/J > 0)\) temperatures [65]. Random quenched dilution of the system relieves the frustration at random localities and can be expected to ordering phenomena at finite temperatures. Indeed, a Monte Carlo study with random quenched dilution of all three sublattices equivalently has indicated spin-glass order [66].

According to conventional mean-field theory, each spin feels an average field, that is, the expectation value, or the thermal average of its neighboring spin \(<s_i>=m_i\), which is not expected to change from site to site, so that it will be everywhere equal to the magnetization. Clearly,

\[ m = \tanh(Jz m), \]
where $z$ is the coordination number.

The mean-field theory of the antiferromagnetic Ising model predicts a phase transition at non-zero temperature even for $d = 1$, whereas the Ising chain has zero magnetization for all $T \neq 0$. In addition, when a phase transition occurs for $d = 2$ or $d = 3$, the theory overestimates $T_c$. Moreover, the critical exponents calculated by means of the theory and the exact Onsager solution are not the same. The fact that every spin behaves in an average, omits the fluctuations in the order parameter. Indeed, it also fails to describe the correlation functions properly in systems with local interactions. It only gives an exact result when the interactions between the spins are infinite-ranged. As a result, the mean-field theory predicts that a given spin feels the effective field determined by the magnetization of its neighbors. This is, however, not the case. In reality, a given spin feels an effective field which is determined by the full spins ($s_i = \pm 1$) of its neighbors.

Recently, Netz and Berker have developed a new mean-field theory which contains the hard-spin condition (i.e., the effect of the full magnitude of each spin) which is essential for frustration and is called the hard-spin mean-field theory [67-77]. According to this theory, a spin $s_i$ that has local magnetization $m_i = < s_i >$, is equal to $-1$ with probability $(1 - m_i)/2 \equiv p_i(-1)$, and to $+1$ with probability $(1 + m_i)/2 \equiv p_i(+1)$. That is,

$$m_i = \tanh(J \sum_j s_j),$$

where $s_j = \pm 1$ with probability

$$p_j(m_j; s_j) = (1 + s_j m_j)/2.$$

Finally, the self-consistent equation for local magnetizations in hard-spin mean-field theory becomes

$$m_i = \left[ \prod_{s_j = \pm 1} p_i(m_j; s_j) \right] \tanh(-J \sum_j s_j), \quad (4.2)$$

where the product and sum over $j$ run over all non-diluted sites neighboring sites $j$. Thus, the spin at each site feels the anti-aligning field due to the full (i.e., hard-) spin of each of its neighbors.

The system is divided into three interpenetrating sublattices which are denoted by $(a, b, c)$. The periodic boundary condition is applied to the system. We
consider the random quenched dilution of the sites of one of three sublattices, let us say, sublattice c. Let \( p \) be the fraction of spins remaining on the diluted sublattice c after the dilution process. Thus, \( p = 0 \) means that all spins belonging to sublattice c are removed, while \( p = 1 \) means that they are all present. In between, the dilution process is random.

After each dilution process with different values of \( p \), the hard-spin mean-field self-consistent equation Eq.(4.2) which is a set of coupled equations for all the local magnetizations is solved iteratively for a given realization of the dilution in a finite but large system. Then, the magnetization of the sublattices, namely \( m_a, m_b \) and \( m_c \), are calculated. During each iteration step, the local magnetizations of all spins on the lattice are calculated.

Alternatively, a further approximation is to average the self-consistent equation over all realizations of quenched site dilution for fixed dilution fraction \( 1 - p \), yielding

\[
m_i = \left[ \prod_j \sum_{\eta_j=0,1} q(p_j; \eta_j) \sum_{s_j=\pm 1} p(m_j; s_j) \right] \tanh(-J \sum_j \eta_j s_j),
\]  

(4.3)

where the quenched-dilution probability distribution \( q(p_j; \eta_j) \) is \( 1 - p_j - \eta_j(1 - 2p_j) \), \( p_j = p_\alpha \) and \( m_j = m_\alpha \) for each sublattice \( \alpha = a, b, c \), and the product and sum over \( j \) run over all sites neighboring site \( i \). Eq.(4.3) is solved for \( (m_a, m_b, m_c) \) for given \( (p_a, p_b, p_c) \). Whereas hard-spin mean-field theory [Eq.(4.2)] yields the variations in the local magnetizations within each sublattice due to differently quenched local environments, the quenched-averaged Eq.(4.3) is a further approximation over hard-spin mean-field theory and, while still incorporating frustration, gives sublattice-wise uniform magnetizations. Eq.(4.3) is a set of three coupled equations, whereas Eq.(4.2) is a set of \( N \) coupled equations, where \( N \) is the number of sites of the system.

4.2. UNSATURATED MAGNETIZATION AND SPIN–GLASS ORDER

Upon random quenched dilution of one sublattice, the frustrated triangular-lattice Ising model does indeed show long-range order, as for example depicted in Figs.4.1. The two undiluted sublattices (labeled a and b), which are now subject to random unfrustrated localities at the dilution points of the other sublattice (labeled c), develop non-zero sublattice-averaged magnetizations, \( m_a = - m_b \),

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at low temperatures. For low dilutions, these magnetizations [Fig. 4.1(a)] show an initial slow growth at onset as temperature is lowered and do not saturate at zero temperature. The diluted sublattice \( c \) is also subject to local liftings of frustration, due to the spatially non-uniform magnetizations of sublattices \( a \) and \( b \). But this is a secondary and, therefore, weaker effect, and sublattice \( c \) does not develop a non-zero sublattice-averaged magnetization. \( m_c = 0 \).

All three sublattices develop, within the ordered phase, non-zero spin-glass order [78], i.e., randomly frozen order, with Edwards-Anderson order parameters

\[
q_\alpha = \left[ \frac{1}{N_\alpha} \sum_i (m_i - m_\alpha)^2 \right]^{1/2},
\]

where \( N_\alpha \) is the number of spins of sublattice \( \alpha \). Note that, for the quenched-diluted sublattice,

\[
q_c = \left[ \frac{1}{N_c} \sum_i m_i^2 \right]^{1/2}.
\]

At high dilutions, the spin-glass ordering trend shows reentrance (as temperature is lowered, increases and then decreases) on the undiluted sublattice [Fig. 4.1(b)] and double reentrance (increase, decrease, and again increase) on the diluted sublattice [Fig. 4.1(c)]. Maximal zero-temperature spin-glass order occurs at intermediate dilutions, as seen in Figs. 4.2(b,c).

The phase diagram of the system is shown in Fig. 4.3. It is seen that a threshold dilution of 4.2% of one sublattice is needed for ordering, i.e., the occupancy \( p \) has to be below 0.958 for ordering. Fig. 4.3 shows the phase boundaries obtained for two realizations of quenched dilutions of a 24 \( \times \) 24 system and the result from averaging over 15 such realizations. Also shown in dashed in Fig. 4.3 is the further approximation of Eq. (4.3). This dashed phase boundary obeys the equation

\[
p^3 f_3 + 3p^2 (1 - p) f_2 + 3p (1 - p)^2 f_1 + (1 - p)^3 f_0 = 4/3,
\]

where

\[
\begin{align*}
f_3 &= (t_6 + 6t_4 + 5t_2)/8, \\
f_2 &= (t_5 + 3t_3 + 2t_1)/4, \\
f_1 &= (t_4 + 2t_2)/2, \\
f_0 &= t_3 + t_1,
\end{align*}
\]

and gives a dilution threshold of 12.5%.
Figure 4.1. Finite-temperature order in the random quench-diluted triangular-lattice antiferromagnetic Ising model: (a) Magnetizations of the two undiluted sublattices from hard-spin mean-field theory (full curves). The curves, with increasing critical temperatures, are for \( p = 0.75, 0.5, 0.09375 \). The result from the further approximation of Eq.(4.3) is given with the dashed curve. The quench-diluted sublattice has zero magnetization. (b) Spin-glass order parameter of the undiluted sublattices. The curves, with increasing critical temperatures, are for \( p = 0.9375, 0.890625, 0.75, 0.625, 0.5, 0.140625, 0.09375 \). Note the reentrant behavior in the magnitudes, for high dilutions. (c) Spin-glass order parameter of the quench-diluted sublattice. The values of \( p \) are as in (b). Here, the spin-glass order for \( p = 0.09375 \) is away from zero only at higher temperatures. The spin-glass order for \( p = 0.140625 \) exhibits doubly reentrant behavior.
Figure 4.2. Zero-temperature sublattice magnetizations and spin-glass order parameters from hard-spin mean-field theory. The sublattice magnetizations (a) do not saturate at zero-temperature, except for the full dilution (hexagonal lattice) limit. The dashed curve in (a) is the result of the further approximation of Eq. (4.3). The zero-temperature spin-glass order (b,c) is maximal at intermediate dilutions. Multiple solutions of the hard-spin mean-field theory equations are seen, in addition to the most stable set depicted in Figs.1. (For each solution, the same symbol is used all of the figures). This figure is obtained for $1/J = 0.0001$, in a $30 \times 30$ system.
Figure 4.3. Phase diagram of the random quench-diluted triangular-lattice antiferromagnetic Ising model. The full curves show the phase boundaries obtained by hard-spin mean-field theory for two different realizations of quenched dilutions of a $24 \times 24$ system. The losanges show the result from averaging over 15 such realizations. The dashed curve is the result from the further approximation of Eq.(4.3); this curve is given analytically by Eq.(4.6).

4.3. A MULTIPLICITY OF ORDERED PHASES AND ORDER PARAMETER OVERLAPS

Within the ordered phase, we find that the hard-spin mean-field equations (4.2) admit, as seen in Figs.4.2,4.4, a multiplicity of solutions, in addition to the set depicted in Figs.4.1. The latter is the most stable solution, in the sense that it has the largest basin of attraction under the iterative solution of Eq.(4.2). The other solutions appear at different temperatures below the onset temperature for the most stable solution. Since, in this study, the number of the sets of solutions increased in going from the $24 \times 24$ system to the $30 \times 30$ system (depicted in Figs.4.2,4.4), it can be inferred that the solutions become numerous in the infinite system.
Figure 4.4. Finite-temperature multiplicity of solutions for $p = 0.75$.

Figs. 4.5, 4.6 depict the overlaps $Q_{\alpha}^{AB}$ between pairs of solutions $(A, B)$,

$$Q_{\alpha}^{AB} = \frac{1}{N_{\alpha}} \sum_{i}^{\alpha} m_{i}^{A} m_{i}^{B}$$

(4.7a)

and the distances $\Delta_{\alpha}^{AB}$,

$$\Delta_{\alpha}^{AB} = \frac{1}{N_{\alpha}} \sum_{i}^{\alpha} (m_{i}^{A} - m_{i}^{B})^{2}.$$

(4.7b)
Figure 4.5. Overlap $Q$ between the different solutions [see Eq.(4.7a)] on the undiluted sublattices, for $p = 0.75$. The arrow indicates the onset of order.

Figure 4.6. Overlap $\Delta$ between the different solutions [see Eq.(4.7b)] on the undiluted sublattices, for $p = 0.75$. The arrow indicates the onset of order. In inset schematizes the distance between the different solutions, showing no ultrametricity.
From $\Delta^A_B$ in Fig. 4.6, we can deduce the separation, in local-order-parameter space, between the different solutions. This is shown schematically in the inset of the figure. We note that the different solutions are not ultrametrically [79] related, since no isosceles-triangle relations are seen. Thus, it may well be that ultrametricity is a property specific to the infinitely connected lattice.

In conclusion, the solution of the hard-spin mean-field self-consistent equations for the fully frustrated antiferromagnetic Ising model on triangular lattice with random quenched dilution yields ordering phenomena after a threshold dilution. The existence of multiplicity of magnetizations for the undiluted sublattices and of spin-glass order parameter for all the sublattices is observed for a given realization of dilution. The dissimilarity index, i.e., the distances $\Delta^A_B$ obeys no ultrametricity.
5. DISCUSSION

Our studies on two athermal and one thermal systems containing annealed and quenched randomness give rise to interesting questions and point to promising avenues of further research, which we would like to discuss here.

The adsorption–reaction model can be related to a kinetic Ising model describing the roughening of a line of separation between two pure phases in two dimensions [61]. The occupied sites then correspond to, say, up spins and the vacant sites to down spins, and each possible interfacial configuration can be mapped uniquely to such a spin configuration. Clearly, for finite surface tension $\sigma_t$ (which is proportional to the free-energy cost per unit increase in the “chemical length” along the interface), the surface thickness $y_L$ is finite. This situation corresponds to the $\epsilon \neq 0$ region in our model.

As $\epsilon \to 0$ we encounter the situation that the interface length grows without bound, and in fact the interface becomes an isotropic fractal with $D_f \simeq 1.8$. The interfacial fluctuations therefore have power–law correlations. This is similar to the behavior of the Ising interface near the critical point, where the surface tension also goes to zero, with a power law dependence on $(T - T_c)$. (It should be remarked that the surface tension also goes to zero as $T \to \infty$, and the interfacial length diverges there; however there the correlations decay exponentially). If the interface thickness is identified with the correlation length, and if one makes the simplest assumption that $\epsilon \propto T - T_c$, then one sees that the Ising model in two dimensions yields a different value for the thickness exponent, namely, $\nu = 1$, not equal to $1/2$. It is of great interest to see if the two models are indeed in different universality classes or whether they can be mapped onto each other, even though the dynamics of the adsorption–reaction model seems to be completely different.

It should be mentioned that the reaction region can be described by stochastic differential equations of the multiplicative noise type with a single component field, namely, the Langevin equation, since in our model interface sites cannot be created spontaneously either in the bulk or in the vacant region. Then, by using dynamical renormalization group, the $\epsilon$–expansion techniques, etc., one may obtain the critical exponents. It has been claimed out by Tu, Grinstein,
and Muñoz [80] that the critical behavior of such systems should be obtainable from the KPZ equation. It would also be possible to do some mean-field like approximation, for instance, mean-field renormalization, for the rate of island production, the diffusion constants of the islands and lakes, and the width of the interface, in order to investigate critical exponents we found from the simulations.

The application of the hard-spin mean-field theory to the antiferromagnetic Ising model on triangular lattice with random quenched disorder gives a multiple set of solutions with a limited number. As it can be seen from Fig.4.2 that each solution does not follow a line continuously. We believe that these are finite-size effects. That is, if one increases the size of the system, it would be possible to find more solutions, each of which may exhibit a continuous line.

Moreover, our set of solutions does not obey ultrametricity. In fact, this is not the case for the mean-field results of the system containing infinite-range interactions. It is still an open question whether multiple solutions of systems with short-range interactions show ultrametricity or not. For this, it will be very interesting to apply hard-spin mean-field theory to different kind of frustrated systems, for instance, where the interactions $\pm J$ are distributed randomly. It would be of great utility to extend the applicability of the hard-spin mean-field theory to non-equilibrium dynamical systems exhibiting phase transitions, in particular, to the aging of spin-glasses. In this way it may be possible to directly monitor the lifting of the multiplicity of solutions.

Another field where the hard-spin mean-field theory may profitably be applied is self-assembling systems. Self-assembling systems (or, microemulsions), which can be considered as a random surface and mapped into a spin Hamiltonian containing various types of interactions such as diagonal, next-nearest neighbor, and plaquette interactions, exhibit very rich phases. One cannot relate the theoretical results with experiments, and also there is a drastic difference between the results obtained from different analytical approaches, that is, a large number of open questions. I believe that the hard-spin mean field theory can also give accurate results for these systems.
REFERENCES


CURRICULUM VITAE

I borned in 1969 at Afşin. I have completed my primary and high school education in Gaziantep. I have graduated, in 1991, from physics department of Istanbul Technical University (ITU). In 1994, I have obtained M.Sc. degree from Institute of Science and Technology at ITU. I have completed Condensed Matter Diploma Programme at International Center for Theoretical Physics (ICTP), Trieste, Italy in 1995. I have been working at TUBITAK Feza Gürsey Research Institute of Basic Sciences since 1991 as a researcher.