# Theoretical Study of Models For Driven Interface Dynamics

by

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# Abstract

In this dissertation, we review the physics associated with surfaces and interfaces in equilibrium and non-equilibrium. Our emphasis will be on interfaces that are driven far away from equilibrium with special interest in the phenomenon of kinetic roughening. Models which describe non-equilibrium interfaces will be introduced and analyzed using techniques such as the Renormalization Group, Monte Carlo simulations, and direct integration of the equation of motion. Different interface relaxation mechanisms will be discussed with a focus on surface diffusion, which is believed to be the dominant effect in Molecular Beam Epitaxy. These interface growth models generate self-affine structures with various correlations satisfying a dynamic scaling law. We compute the scaling exponents and functions. Finally, we study the effect of quenched impurities on the dynamics of a driven interface with a conservation law. The impurity effect leads to anomalous scaling exponents and qualitatively changes the interface dynamics. Our results are summarized in two articles to be published: Refs. (Govind and Guo, 1992; Govind, Guo and Grant, 1992).

# Résumé

Dans cette dissertation, nous passons en revue la physique associeé aux surfaces et aux interfaces aussi bien en état d' équilibre que hors d'équilibre. Nous étudions plus spécialement, les interfaces qui sont dans un état eloigné de l' équilibre en portant un interêt particulier au phénomène de cinétique rugueuse. Les modèles décrivant les interfaces hors d'équilibre seront introduits et analysés à l'aide de techniques tels le groupe de renormalisation, les simulations de Monte Carlo, et l'intégration numérique de l'équation de mouvement. Nous discutons deux mécanismes de relaxation et considérerons l'effet de diffusion de surface que l'on croit prédominant dans les expériences de "Molecular Beam Epitaxy". Ces modèles de croissance d'interfaces produisent des surfaces à géométrie affine, dont les corrélations satisfont aux lois d'échelle dynamiques. Nous calculons ces fonctions ainsi que les exposants critiques. Finalement, nous étudions l'effet d'impurités sur la dynamique d'interfaces hors d'équilibre, contrôlée par une loi de conservation. Les impuretés changent qualitativement la dynamique et produisent des exposants d'échelle anormaux. Nos résultats seront publiés dans deux articles: Refs. (Govind et Guo, 1992; Govind, Guo et Grant, 1992).

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# Chapter 1

# Introduction

Interfaces play a very important role in physics, chemistry, engineering, biological systems, etc. They have fascinated scientists for many years, who have tried to unravel their various properties. We shall only be looking at interfaces as they occur in condensed matter systems such as the surfaces of solids, liquids... In condensed matter physics, the study of interfaces in conjunction with the physics of phase transitions have produced many interesting results. The roughening transition is one beautiful example. This problem has been the centre of intense study for a number of years beginning with the work of Burton, Cabrera and Frank(1951)(Burton, Cabrera and Frank, 1951), who conjectured the existence of a roughening transition in an equilibrium interface. The problem has since been studied by a large number of authors and as it stands has been well understood.

Interfaces are rarely found in equilibrium. They occur mainly in non-equilibrium systems such as snowflakes, some quenched crystals, surfaces of dendrites, etc. This makes their study much more complicated than the more straight forward equilibrium situation. Since a lot of attention has been channeled into systems near or at equilibrium, systems far away from equilibrium were largely neglected. These systems are more realistic as they include many more physically relevant parameters, for example it has been found that driven systems have a higher roughening temperature when compared to systems that are not.

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Over the last few years many models have been constructed to investigate nonequilibrium interfaces in finer detail. The single significant contribution in the last decade has been the work of Kardar, Parisi and Zhang (1986) (Kardar, Parisi and Zhang, 1986; Medina et al., 1989) who developed a non-linear stochastic differential equation to model a growing interface driven by an external flux of particles. We shall get back to the KPZ equation and understand it in greater detail later on in the chapter. Non-equilibrium interface problems have also been addressed from a numerical viewpoint using Langevin simulations(Guo, Grossmann and Grant, 1990a; Amar and Family, 1990), Monte Carlo techniques(Kim and Kosterlitz, 1989; Roland and Guo, 1991; Guo, Grossmann and Grant, 1990b; Sarma and Tamborenea, 1991) and other numerical models like cluster growth models, etc(Vold, 1959; Vold, 1963; Meakin and Family, 1986; Ramanlal and Sander, 1985; Krug and Spohn, 1990; Vicsck, 1989; Family and Vicsek, 1991). The remainder of the chapter is organized as follows: we shall consider free interfaces in equilibrium and interface fluctuations, interfaces in the presence of external fields will then be considered. We shall conclude this introductory chapter with a discussion of some non-equilibrium growth processes, the understanding of which will be our focus for the remainder of this dissertation. A note about notation used, spatial dimension d would be referred to as  $d_I + 1$ , where  $d_I$  is the interface dimension.

# 1.1 Free interfaces in equilibrium and interface fluctuations

An interface in the strict sense is the boundary between two bulk phases say A and B coexisting in equilibrium (Wortis, 1985). Equilibrium implying that the bulk phases A and B be separated in a phase diagram by a first-order phase boundary and that all the relevant parameters be adjusted such that the system always lies on this boundary Fig. 1.1. Single interfaces may be studied both in the presence and absence of external fields (free interfaces). In writing down a theoretical model there are various

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Figure 1.1: Typical phase diagram of a gas-solid-liquid system. All the phase boundaries shown are first order.

approaches one may adopt, the three main ones being,

(a). models purely based on the microscopics and using a microscopic Hamiltonian.

(b). density functional theories

(c). interface Hamiltonians which are basically functionals of the local departure from the interface.

On scales larger than the molecular size but smaller than the overall size of the system, interfaces do not have a fixed shape. Fluctuations present in the system make them undulate and these shape fluctuations lead to an interfacial roughness. These undulations do not preserve the total area of the interface and are in general governed by an interfacial tension or stiffness. In the case of a liquid-vapour system these excitations or fluctuations represent capillary modes. For a crystal-vapour interface, these shape fluctuations are constructed from microscopic steps or ledges which separate atomically flat terraces on the surface. At finite temperatures T > 0, interfaces fluctuate to increase their entropy. Interfacial fluctuations may also be caused by the presence of quenched random impurities in the system. In this case the interface fluctuates to adapt its shape to the background randomness in an effort to minimize



Figure 1.2: A boundary line in d = 1 + 1 dimensions.

its energy.

Studying interfaces therefore basically boils down to studying interface fluctuations discussed in the previous paragraph. As already mentioned interfaces may be studied from a microscopic, density functional and interfacial Hamiltonian viewpoint. In principle each of these approaches should very well be capable of handling interfacial fluctuations as well. It turns out that most methods are often very difficult to handle and the effective interfacial Hamiltonian method is the one most commonly used.

We shall begin our 'interfacial fluctuations' voyage with an understanding of a simplified model - the liquid-vapour interface(Ma, 1980). For simplicity we shall start with a two-dimensional system, assuming that the energy of the boundary between the liquid and vapour phases is proportional to its length we have,

$$H_I = \nu L \tag{1.1}$$

where  $H_I$  is the interfacial energy,  $\nu$  is the surface tension and L is the length of the interface, Fig. 1.2.

#### **INTRODUCTION**

7 1 Using the above figure,

$$L = \int_0^{L_{\bullet}} [1 + (\frac{dz}{dx})^2]^{1/2} dx$$
 (1.2)

If the gradients are small i.e. for slowly varying steps,  $\frac{dz}{dz} \ll 1$  we may expand the term in the square brackets to first order,

$$L \simeq L_o + (\frac{1}{2}) \int_0^{L_o} (\frac{dz}{dx})^2 dx$$
 (1.3)

Fourier decomposing z(x),

$$z(x) = \left(\frac{1}{L_o}\right)^{1/2} \sum_{k} z_k \exp(ikx)$$
(1.4)

Substituting (1.4) into (1.3) we find,

$$L = L_o + (\frac{1}{2}) \sum_{k} k^2 |z_k|^2$$
(1.5)

Using the equipartition theorem,

$$\nu k^2 |z_k|^2 = T \tag{1.6}$$

where we have set the Boltzmann constant to 1.

Defining  $\Delta z = z(x) - z(x')$  as a measure of the wandering of the interface,

$$<(\Delta z)^2>=2< z^2>-2< z(x)z(x')>$$
 (1.7)

i.e,

$$= \left(\frac{T}{\pi\nu}\right) \int_{-\infty}^{+\infty} dk \frac{1}{k^2} [1 - \cos k(x - x')]$$
(1.8)

$$=\frac{2T}{\nu}(|x-x'|)$$
(1.9)

For  $|x - x'| \sim L_o$ ,  $\langle (\Delta z)^2 \rangle \sim (T/\nu)L_o$ . The thickness of the interface  $\sim (\langle (\Delta z)^2 \rangle)^{1/2}$  thus goes as  $\sqrt{L_o}$ , diverging as  $L_o \to \infty$ . The boundary line is therefore 'rough' and not 'smooth'. In technical terms these long wavelength modes that make the interface slosh back and forth are called Goldstone modes.

The above discussion may be easily carried over to higher dimensions. In three spatial dimensions for example one has a two dimensional surface. The energy in this case would now be proportional to the area of the interface.

$$H_I = \nu A \tag{1.10}$$

where,

$$A = \int d^2 r [1 + (\nabla z)^2]^{1/2}$$
 (1.11)

Using the same assumptions as before we have,

$$H_I \simeq L_o^2 + (\frac{1}{2}) \int d^2 r (\nabla z)^2$$
 (1.12)

Therefore  $< (\Delta z)^2 >^{1/2}$  goes as,

$$\sim \frac{T}{\pi\nu} \frac{\ln|r-r'|}{a} \tag{1.13}$$

where a is approximately the interatomic distance. For large |r - r'|, the interface is therefore rough no matter how low the temperature is. The model of the free interface that we have analyzed so far makes the implicit assumption that the material in question is a continuous one, and that the interface is elastic in nature. This description turns out to be quite accurate in describing the liquid-vapour system. However, if we had a crystal-vapour system the discreteness of the lattice would have to be incorporated. We shall examine this in a later section. Another important factor that was neglected in the preceding discussion was the effect of gravity. This and the effects of other external fields would be considered in the next section.

## **1.2** Interfaces and external fields

So far we have only considered free surfaces. The next thing to do would be to introduce an external field and study how interfaces and their fluctuations respond (Fisher, 1989). These external fields may be (a). slowly varying

(b). periodic

(c). quasi-periodic

(d). random

We shall study the effect of each one of these fields in brief.

#### **1.2.1** Slowly varying fields

The gravitational and van der Waalsian forces are two examples of slowly varying fields. We shall only consider the gravitational force here, the van der Waals force may be treated in a similar manner. Gravity as we all know is a very weak force, it nevertheless is responsible in keeping a liquid-vapour interface horizontal. When a liquid surface rises by an amount z, it produces hydrostatic pressure  $\rho g z$ , where  $\rho$  is the difference  $\rho_l - \rho_g$ ,  $\rho_l$  being the density of the liquid and  $\rho_g$  the density of the gas. Hence, the energy associated with it would be  $\frac{\rho g z^2}{2}$ . This extra contribution would have to be added to the free interface Hamiltonian  $H_I$  we discussed in the previous section (Buff, Lovett and Stillinger, 1965). Therefore,

$$H_I = L_o^2 + \frac{\nu}{2} \int d^2 r [(\nabla z)^2 + \frac{z^2 \rho^2 g^2}{\nu}]$$
(1.14)

The average density profile may be calculated using the equilibrium distribution,

$$P(z) \sim \exp[-\frac{H(z)}{T}]. \tag{1.15}$$

The width  $< (\Delta z)^2 >^{1/2}$  is consequently given by,

$$< (\Delta z)^2 >^{1/2} = \left[\frac{T}{4\pi\nu}\ln(1+\frac{L_c}{l})\right]^{1/2}$$
 (1.16)

where  $L_c$  is the capillary length,

$$L_{c} = \left[\frac{\nu}{g\rho}\right]^{1/2} \tag{1.17}$$

and  $\rho = \rho_l \sim \rho_g$ . *l* is the length scale such that the correlations over distances smaller than *l* are no longer described by capillary wave theory. This capillary wave model thus predicts that the interfacial width diverges when  $g \rightarrow 0$ ,

$$< (\Delta z)^2 >^{1/2} \sim [\ln g]^{1/2}$$
 (1.18)

This divergence occurs despite the stabilizing effect of the surface tension. The analysis on the van der Waals force is exactly the same as in the gravitational case(Bedeaux, 1985).

### 1.2.2 Periodic potential

Let us now consider an interface which separates a periodic crystalline phase with lattice constant  $a_o$  from another phase. In this situation, the interface feels an effective potential V(z) due to the underlying periodicity of the crystal lattice. The potential could be of the form

$$V(z) = -\overline{A}\cos(kz) \tag{1.19}$$

where  $\overline{A}$  is a constant inversely proportional to temperature  $(\overline{A} = \frac{A}{T})$  and  $k = \frac{2\pi}{a_{\bullet}}$ . Having defined the potential, we can now construct an effective Hamiltonian to describe the interfacial configuration.

$$H_I(z) = \int \frac{(\nabla z)^2}{2\overline{T}} + V(z)$$
 (1.20)

where  $\overline{T} = \frac{T}{\nu}$ .

The above model is identical to the sine-Gordon Hamiltonian and in 2 + 1 dimensions leads to a roughening transition at a finite temperature  $T_r$  (Chui and Weeks, 1976; Weeks, 1984) which has been shown to be of the Kosterlitz-Thouless (KT)(Kosterlitz, 1974) type. It was found that for temperatures  $T > T_r$ , the periodic potential V(z) is irrelevant and the surface is always rough, while for temperatures  $T < T_r$  the potential is relevant and causes the interface to remain smooth. When  $T \rightarrow T_r$  from below, we encounter a phase transition from the smooth to the rough phase. However, in d = 1 + 1 the above periodic potential is totally irrelevant for all finite T > 0, the surface is always rough. We thus have no phase transition in d = 1 + 1 dimension.

#### 1.2.3 Quasi-periodic potential

Suppose the crystalline phase under consideration was quasi-periodic rather than periodic. We would have to define a new potential, for example

$$V(z) = -A_o \cos(k_o z) - A_1 \cos(k_1 z)$$
(1.21)

where  $\frac{k_o}{k_1}$  is an irrational number. The interface Hamiltonian as before would be

$$H_I(z) = \int \frac{\nu(\nabla z)^2}{2} - A_o \cos(k_o z) - A_1 \cos(k_1 z)$$
(1.22)

It has been shown recently by Lipowsky and others (Lipowsky and Henley, 1988; Henley and Lipowsky, 1987; Garg and Levine, 1987)that in d = 2 + 1 the above Hamiltonian leads to a smooth interface for all  $T < \infty$ . In d = 1 + 1 however, the behaviour is non-universal and depends on the precise form of the quasi-periodic potential. For the potential considered above, one gets a second order roughening transition in d = 1 + 1. In general they (Lipowsky and Henley) found very different interfacial behaviours for random and ideal quasi-crystals, the ideally tiled case had a roughness that was lesser than the random case in both two and three dimensions.

#### 1.2.4 Random potential

When a system contains quenched random impurities, these objects may in general be modeled using random fields or bonds (Grinstein and Ma, 1982; Villain, 1982; Nattermann and Renz, 1988; Huse, Henley and Fisher, 1985; Kardar, 1985; Huse and Henley, 1985). An interface, when it interacts with such an environment would try to adapt its shape to the effective random background potential in order to minimise its energy and consequently increases its roughness at finite T (T > 0). There are other problems as well that can be studied when one has a random potential such as the localization-delocalization of an interface. When one has an attractive potential  $V_{e}$ , the interface in the random environment may be localized and as one decreases the strength of this potential the interface delocalizes itself. As before the interfacial

#### INTRODUCTION

fluctuations may be described using an effective Hamiltonian,

$$H_I(z) = \int \frac{\nu(\nabla z)^2}{2} + V_1(z)$$
 (1.23)

In principle one can conceive of many other situations. Before we move on, an important point of note is that all the above models share the common property of being effective interface Hamiltonians. Effective interface Hamiltonians in principle should be derived by a systematic coarse graining of a more fundamental lattice model. This procedure is however very difficult to implement in actual practice. One thus resorts to more phenomenological methods like symmetries in the problem to construct the Hamiltonian. In the effective Hamiltonian description, details on length scales smaller than the bulk correlation length are lost. We shall review one of the most widely used lattice models -the Solid-on-Solid(SOS) model in the next section.

## 1.3 Interfaces using Solid-on-Solid models

Lattice models used to describe interfaces form a bridge between the discrete models that deal with the entire system and the continuum models that deal only with the interface. These discrete models contain information regarding quantities such as the transition temperature and they help one study and understand the interactions between the various microscopic parameters better. The most commonly used of all discrete lattice models are the solid-on-solid (SOS) models(Weeks, 1984; Binder, 1983). Before getting into the intricacies of SOS models, we shall first consider the Ising model. The Ising model as we all know consists of a square lattice with a spin  $S_{ij} = \pm 1$  attached to each lattice point. The Hamiltonian can thus be written as,

$$H = -J_1 \sum_{ij} s_{ij} s_{ij+1} - J_2 \sum_{ij} s_{ij} s_{i+1j}$$
(1.24)

where  $J_1$  and  $J_2$  are positive coupling constants in the horizontal and vertical directions respectively. We could choose our boundary conditions in such a way that the top half remains all spin up and the bottom all spin down at T = 0. As we increase the temperature from zero, fluctuations start appearing on the interface and as we £



Figure 1.3: Configurations of the Ising and SOS approximation to the Ising model at finite T. Notice the absence of overhangs and bubbles in the SOS system.

increase the temperature further overhangs and bubbles appear in the system. The connection between the Ising and the SOS models may be made if one neglects the overhangs and bubbles inorder that the fluctuations from the T = 0 configuration remains single-valued. The energy of an SOS interface may then be written as,

$$H \sim J_2 \sum_{k=1}^{L} |z_k - z_{k-1}| \tag{1.25}$$

where we have neglected a constant piece and L stands for the length of the system. Having written out the Hamiltonian, one can easily write out a partition function,

$$z = \sum_{ij} \exp(-\frac{H}{T})$$
(1.26)

which may be evaluated using transfer matrices, recursion relations, direct summation etc. The SOS Hamiltonian has also been recently used to study the phenomena of wetting(Fisher, 1984; Kroll, 1981). Generalising equation.(1.25)

$$H = J \sum_{k} |z_{k} - z_{k-1}|^{p}$$
(1.27)

The above generalisation of the SOS Hamiltonian envelops within it a large number of different cases corresponding to different p's. The discrete Gaussian case corresponds

to p = 2, The restricted solid-on-solid model(RSOS)(Kim and Kosterlitz, 1989) to  $p = \infty$  and the anisotropic Ising model to p = 1. The above model when analyzed in d = 1 + 1 dimensions (1 interface dimension) does not show any phase transition at finite temperatures: the interface is always rough. A well defined transition or roughening temperature however exists in d=2+1 dimensions(Mon *et al.*, 1988). The above discussion was merely an introduction to the idea behind most SOS models. A large number of them may be solved exactly with and without interactions. As for the remaining that cannot be tackled analytically, they have been studied numerically using Monte Carlo simulations. So far we have studied models that are basically governed by a Hamiltonian. The Hamiltonian as we very well know helps describe only the 'static' properties of a system. In other words one can understand the equilibrium properties very well with a well defined Hamiltonian. The next pertinent question is: what happens when there are growth processes involved which are characterised by a dynamics that is far away from equilibrium ?. Such systems cannot be described using a Hamiltonian.

# 1.4 Non-equilibrium growth processes

In nature there are a large number of non-equilibrium processes that give rise to interfaces far from equilibrium. We shall review a few of them in brief in this section.

## 1.4.1 Sputter Deposition

As we all know coatings play an important role in many daily life applications. Typical examples are Teflon coats on utensils, coatings on sunglasses etc. Sputter deposition that we shall describe here is just one way a coating can be made. This method involves the deposition of energetic atoms or ions onto a growing surface. The incoming atoms travel along ballistic trajectories, mostly along the normal to the substrate. The atoms or ions once they deposit themselves on the surface move around till they find a suitable site where they coalesce and form tiny microcrystallites. These micro-



Figure 1.4: Schematic diagram showing the various zones.

crystallites are very small if the temperature is low, this results in the amorphous nature of the film for any deposition rate(Vossen and Kern, 1978; Bruinsma, Karunasiri and Rudnick, 1990). The non-equilibrium nature of these films causes them to develop very complicated surface morphologies which can be classified according to the structure zone model(SZM) developed by Movchan and Demchishin(Movchan and Demchishin, 1969). The model distinguishes three different zones.

(a). columnar

(b). surface diffusion mediated zone

(c). bulk diffusion and recrystallization zone

depending on the ratio  $\frac{T}{T_m}$  where T is the temperature of the substrate and  $T_m$  is the melting temperature of the bulk adsorbed material. The boundaries of these zones are regions of low adatom density and they play a significant role in determining the transport and mechanical properties of the material. It turns out that if temperatures are elevated beyond a certain maximum temperature, bulk diffusion of matter sets in and results in thermal roughening making the process highly sensitive to te nperature. Closely related to the sputter deposition process is the sputter erosion process. It is infact the inverse process. The evolution of macroscopic features during erosion



Figure 1.5: Actual configurations of sputter deposited films.

and etching have been extensively studied and it has been observed that the surface is covered with cones and ridges.

#### 1.4.2 The Molecular Beam Epitaxial Process

Molecular Beam Epitaxy (MBE) is a method of growing thin films, that distinguishes itself from other vacuum evaporation techniques in that one has a more control over tha beam and the deposition conditions (Chang and Ploog, 1985). As a result, the films grown this way have much better electrical and optical properties than ones grown by conventional means. This technique has been used to fabricate semiconductor, metal, insulator thin films etc. The MBE growth process involves the reaction of one or more thermal beams of atoms or molecules with a crystalline surface under high vacuum conditions at temperatures around 900 - 1100K which is much lower than the temperatures required for a chemical vapour deposition process. The important feature of a MBE process is that the growth rate of the crystal remains a constant for a wide temperature range. The typical MBE growth process my be split into two parts. The first step involves the deposition of the atom onto the substrate, and the second involves its incorporation. The second step is normally achieved by



Figure 1.6: Typical MBE growth showing the crystal growing in an oscillatory manner.

surface diffusion over the surface to a suitable growth site, a step or a kink. Since the atom always chooses a step or a kink, the step flow is an important growth mechanism. At the above mentioned temperatures where MBE is normally performed, the incoming atoms and the substrate have different temperatures. This results in a typical non-equilibrium situation, which gives rise to flux or current causing the atom to move around on the surface. In other words, if the time in which the atom has to find itself a suitable site in the 'energetic sense' is quite small, the liklihood of it finding one would be rather slim. Typically the atom makes a large number of attempts before it settles down on the surface, making the relaxation time rather large, thus delaying the onset of equilibrium. It has been observed using reflection high energy electron diffraction (RHEED) that at temperatures that are fairly high, and when the surface is parallel to a high symmetry orientation, the roughness of the surface oscillates and exhibits minima separated by maxima with the minima corresponding to the successive completion of layers. The continuum models that we shall develop in the next chapter will not account for this oscillatory behaviour in the roughness but will give us a picture of the interface roughness over larger length scales.

# 1.4.3 Interfaces resulting from the immiscible displacement of viscous liquids in porous media or in the presence of a quenched random medium

Recent experiments (Rubbio et al., 1989; Rubbio et al., 1990; Martys, Cieplak and Robbins, ) conducted on the time evolution of the geometry of rough interfaces generated by fluids flowing through a porous medium have shown that these interfaces exhibit dynamic scaling and self-affine structures. This displacement of one fluid by the other depends intimately on the viscosities and the wetting properties of the media involved. In these experiments the displacing liquid is chosen such that it preferentially wets the medium, the liquid thus moves through smaller pores at lower pressures than those required to move through larger ones. This causes certain sections of the interface to move more easily and consequently more rapidly than others. The fluid interface is said to be pinned at the larger pores. We shall investigate this phenomenon in greater detail in Chapter 5.

In Chapter 2, we shall review the scaling property of growing interfaces and physical aspect of various relaxation mechanisms that attempt to bring a growing interface back to equilibrium. Models both discrete and continuum will be developed to illustrate these ideas. Chapter 3 will provide an illustration of the Renormalization Group method as applied to statics and dynamics. We shall then go on to apply both numerical and exact analytic techniques to study a certain surface diffusion dominated continuum model(Govind and Guo, 1992) in Chapter 4. The effects of quenched impurities on the dynamics of interfaces(Govind, Guo and Grant, 1992) will be taken up in Chapter 5. We shall end with a conclusion in Chapter 6.

# Chapter 2

# Models of Dynamically Growing Rough Interfaces

Dynamically growing interfaces have been successfully studied over the past several years using various models, numerical as well as phenomenological equations of motion (Kardar, Parisi and Zhang, 1986; Villain, 1991; Wolf and Villain, 1990; Edwards and Wilkinson, 1982; Sun, Guo and Grant, 1989; Lai and Sarma, 1991; Golubovic and Bruinsma, 1991). In this chapter, before we review suitable examples from both approachs, we shall first study an important property inherent to all non-equilibrium growing interfaces, the scaling property. This property as we shall see later would enable us use powerful field theoretic techniques commonly used in critical phenomena, to study these interface problems.

# 2.1 Scaling properties of growing interfaces

Studies on growing interfaces have revealed that these objects have fractal like forms and evolve into a steady-state having no characteristic length and time scales. Technically such a system would be termed as 'scale-invariant'. The dynamical scaling aspect has been studied by a large number of authors over the last decade. We shall highlight the formalism due to Family and Vicsek(Family and Vicsek, 1985) which is based on the scaling of the interface width. Any interface in general may be described using the interfacial height h(x, t) measured from the t = 0 position (initial flat interface). A limitation of this description is that the height must be single-valued (free from bubbles, overhangs, etc). We may define an average height at some arbitrary time t as,

$$< h(x,t) >= \frac{\sum h(x,t)}{L^{d-1}}$$
 (2.1)

The interfacial height fluctuations from the above average value gives us a measure of the interfacial thickness or the width. The width or thickness is then defined as,

$$W(L,t) = [\langle h^2(x,t) \rangle - \langle h(x,t) \rangle^2]^{1/2}$$
(2.2)

which is essentially the standard deviation of the height fluctuations. Empirical studies on interface fluctuations have revealed the inherent scale-invariant nature of interface growth. These studies have shown that one can in general expect the width W(L,t) to grow in time as some power of t.

$$W(L,t) \sim t^{\beta} \tag{2.3}$$

where the exponent  $\beta$  helps characterise correlations in time. Correlations in space on the other hand are constrained by the linear size of the system, L. Once the correlations have reached this length, they cannot extend further, the interface at this point attains a steady-state value and is characterised by a constant value for the width. The interface being scale invariant can once again be described by a power law but now in L,

$$W(L, t \to \infty) \sim L^{\alpha}$$
 (2.4)

where  $\alpha$  is normally referred to as the 'wandering' or 'roughness' exponent(Fisher, 1986). Rough surfaces normally have  $0 < \alpha < 1$ . An  $\alpha = 0$  is characteristic of two dimensional surfaces in thermal equilibrium and some other non-equilibrium systems such as critical faceting, etc. In this case the power law is replaced by a 'log' like

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behaviour,

$$W \sim (\log L)^{\alpha'}. \tag{2.5}$$

Interfaces with  $\alpha = 1$  have at least in equilibrium cases been associated with the breakdown of two-phase coexistence at the lower critical dimension(Huse, Henley and Fisher, 1985; Fisher, 1986). In this case, one would have to abandon the single-valuedness of the interfacial height h(x, t) and allow the possibility of bubbles and overhangs. An SOS description of the problem would consequently breakdown. There have a number of investigations regarding non-equilibrium cases as well.

Combining equations.( 2.3) and ( 2.4) we can get a homogenity relation for dynamical scaling,

$$W(L,t) \sim L^{\alpha} f(\frac{t}{L^{*}})$$
(2.6)

where  $z = \frac{\alpha}{\beta}$ , this exponent helps describe the scaling of the correlations in the transverse direction of the surface. The exponents  $\alpha$  and  $\beta$  may also be defined using the height difference correlation function C(x, t) given by,

$$C(x,t) = \langle [h(x,t) - h(0,0)]^2 \rangle_{x,t}$$
(2.7)

$$C(x,0) \sim x^{2\alpha} \tag{2.8}$$

for  $x \ll L$ , and

$$C(0,t) \sim t^{2\beta} \tag{2.9}$$

for small times.

## 2.2 Numerical Models

Numerical models differ from continuum ones in that they are actual experiments performed on a computer. In other words the actual physical process is mimicked



Figure 2.1: Interface grown by random deposition of particles.

using simple rules. These models are useful as they deal with the fundamental building blocks governing the process. In this section we shall discuss some extensively studied numerical models, that have helped shed light on the fundamentals of the non-equilibrium crystal growth process thus paving the way for continuum descriptions that we will discuss in the next section. We shall review three models.

- (a). random deposition models
- (b). ballistic deposition
- (c). the eden model

## 2.2.1 Surface growth by random deposition (RD)

This model (Vold, 1959; Vold, 1963) is simulated by raining particles down on to a substrate: a point is randomly selected above the substrate and a particle is allowed to fall vertically down along a straight line from here. The result of this is the formation of long columns. Since the particles are dropped at random, we have no correlations among the columns. The width  $W(L, t) \sim t^{1/2}$  regardless of the dimension in which the experiment is performed. The width in other words performs a random walk.



Figure 2.2: A ballistically grown interface.

#### 2.2.2 Ballistic deposition (BD)

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The particles in this model are released from randomly chosen launching points and move along parallel straight lines till they encounter the aggregate to which they attach themselves. The angle of incidence of the launched particles may be varied. In actual practice, one defines a substrate length L. The launching points are chosen at random at a height just above the maximum of the deposit. The launched particle travels along a straight line, the moment it makes contact with another particle in the substrate, it becomes a part of the collection already deposited. This model shows non-trivial scaling in contrast to the to the random deposition model, and the growing aggregate has a number of holes and overhangs present in it. The width W(L,t) scales like  $t^{1/3}$  in time and goes as  $L^{1/2}$  with the size of the system(Jullien and Meakin, 1987). The difference in exponents can be attributed to the fact that growth in the BDM takes place normal to the local interface where as it takes place normal to the original substrate in the RD case.



Figure 2.3: Compact structure of the Eden model.

#### 2.2.3 Eden Model (EM)

Eden(Eden, 1961) in 1961 introduced this model to study the dynamics of tumor growth. The growth algorithm in this case consists in choosing a single perimeter site at random and filling it with a probablity of  $\frac{1}{N}$ , where N is the number of perimeter sites available. Therefore in a given time step each nearest neighbour of the cluster has the same probablity of being filled. This growth model leads to compact d dimensional objects that have a non-trivial surface structure. Compact, meaning that there are no overhangs and bubbles. Many different versions of this model have been studied(Jullien and Botet, 1985; Freche, Stauffer and Stanley, 1985) we shall merely quote results here.

(a). d = 2,  $\beta = 0.33$  and  $\alpha = 0.5$ .

(b). d = 3,  $\beta = 0.22$  and  $\alpha = 0.33$ .

(c). d = 4,  $\beta = 0.15$  and  $\alpha = 0.24$ .

## 2.3 Continuum equations of crystal growth

Phenomenological or continuum approaches are normally based on langevin equations of motion. In constructing these equations only the essential terms relevant to the physical process are considered. Loosely speaking these equations can in principle be derived by a systematic coarse graining of certain discrete models like those discussed in the previous section. However, this procedure as already mentioned is difficult to implement. We shall not use this approach, but instead use one which looks at things from a 'macroscopic' perspective. As we have already seen, films are normally grown using techniques like vapour deposition, MBE etc. In other words, by depositing atoms onto a substrate in a controlled manner. If these deposited atoms are somehow prevented from moving around on the substrate, the surface would become extremely rough and this would result in the amorphisation of the material and thus form bad crystals. The recovery mechanisms that help us get around this problem are,

- (a).desorption or evaporation
- (b).surface diffusion
- (c).volume diffusion

(d).vacancy formation in the superficial layers

to name a few. Of these only surface diffusion and surface desorption will be considered. It will be implicitly assumed that the average surface is orthogonal to the direction of increasing height.

#### 2.3.1 Desorption or evaporation dynamics

Consider an curve y(x) between two points A and B, to be a portion of the interface between a solid and a fluid phase (Mullins, 1963; Mullins, 1957; Mullins, 1959; Landau and Lifshitz, 1967). The free energy F(x) in one dimension as we have already seen can then be written as,

$$F=\int_{A}^{B}\sigma ds,$$

$$=\int_{A}^{B}\sigma\sqrt{1+\dot{y}^{2}}dx.$$
 (2.10)

where  $\dot{y} = \frac{dy}{dx}$ . Let us now perturb the y(x) by a small amount, i.e

$$y'(x) = y(x) + \delta y(x) \tag{2.11}$$

the variation  $\delta y$  is considered small. The variations at the end-points  $\delta y(A)$  and  $\delta y(B)$  are taken to be zero and  $\int_{A}^{B} \delta y(x) = 0$ . Using calculus of variations, it can be shown that the corresponding variation in the free energy  $\delta F$  is,

$$\delta F = \int_{A}^{B} \frac{dG}{dy} \delta \dot{y} dx,$$
  
= 
$$\int_{A}^{B} \frac{dG}{dy} \frac{d}{dx} \delta \dot{y} dx,$$
  
= 
$$-\int_{A}^{B} \frac{d}{dx} \frac{dG}{dy} \delta \dot{y} dx.$$
 (2.12)

after integrating by parts, with  $G(\dot{y}) = \sigma(\dot{y})(1+\dot{y}^2)^{\frac{1}{2}}$ . We also have,

$$\delta F = \frac{1}{\Omega} \int_{A}^{B} \mu \delta y dx. \qquad (2.13)$$

where  $\mu$  is the chemical potential,  $\Omega$  is the atomic volume and  $\frac{\delta y dx}{\Omega}$  is the number of atoms that get included when we make the infinitesimal change in the interfacial function y(x). We thus have two expressions for the change in the free energy. Subtracting one from the other we get,

$$\mu = -\Omega \frac{d}{dx} \frac{dG}{d\dot{y}},\tag{2.14}$$

and substituting back for  $G(\dot{y})$ ,

$$\mu = -\Omega \frac{d}{dx} \left( \frac{d}{d\dot{y}} (\sigma(\dot{y})(1+\dot{y}^2)^{\frac{1}{2}}) \right).$$
(2.15)

Using,

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$$\frac{d\sigma}{d\dot{y}} = \frac{1}{1+\dot{y}^2} \frac{d\sigma}{d\theta},\tag{2.16}$$

where  $\theta = \arctan \dot{y}$ , therefore,

$$\mu = -\Omega\left(\sigma + \frac{d^2\sigma}{d\theta^2}\right) \frac{\ddot{y}}{\left(1 + \dot{y}^2\right)^{\frac{3}{2}}},$$

$$= \Omega\left(\sigma + \frac{d^2\sigma}{d\theta^2}\right) K$$
(2.17)

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where K is the curvature at the point in question reckoned positive when the the surface is concave,  $\mu = 0$  evidently corresponds to a flat surface (K = 0). The above expression clearly holds only for orientations at which the second derivative of  $\sigma$  exists(it does not hold for cusps). We could generalise the above expression for dimensions greater than d = 1 + 1. For two different principal curvatures  $K_1$  and  $K_2$ , the above expression may be generalised to,

$$\mu = \Omega[(\sigma + \frac{d^2\sigma}{d\theta_1^2})K_1 + (\sigma + \frac{d^2\sigma}{d\theta_2^2})K_2]$$
(2.18)

If  $\sigma$  is isotropic, as in a liquid, the angular derivatives vanish resulting in,

$$\mu = \Omega \sigma [K_1 + K_2] \tag{2.19}$$

which is the classical Gibbs-Thomson formula. Recalling the definition of the curvature,

$$K = \frac{\nabla^2 h}{(1 + (\nabla h)^2)^{\frac{3}{2}}}$$
(2.20)

and for small gradients,

$$K \approx \nabla^2 h \tag{2.21}$$

Therefore,

$$\mu \propto \nabla^2 h \tag{2.22}$$

In other words, the chemical potential is proportional to the curvature. Assuming the chemical potential of the vapour  $(\mu_v)$  to be a constant, the term in the dynamical equation due to desorption can be written as,

$$\frac{\partial h}{\partial t} \propto \mu - \mu_{\nu} \tag{2.23}$$

where  $\mu$  as already described is the local chemical potential at a point. Clearly, the chemical potential cannot contain powers proportional to the first derivatives. If this were so the above dynamical equation would imply a direction dependent growth which is unphysical. Combining the last two equations we get,

$$\frac{\partial h}{\partial t} = \nu \nabla^2 h \tag{2.24}$$

for the deposition process.

#### 2.3.2 Surface Diffusion

In the case of surface diffusion, the transport of material along the surface is given in terms of the Einstein-Nernst equation for the drift velocity v by the expression(Landau and Lifshitz, 1967; Mullins, 1963; Mullins, 1957; Mullins, 1959; Landau and Lifshitz, 1967),

$$J \propto -\nabla \mu$$
 (2.25)

where the derivative is taken along the surface because the slope is small. Since  $\mu$  is proportional to the local curvature of the surface, the above equation becomes

$$J \propto \nabla \nabla^2 h,$$
 (2.26)

and since the total mass is conserved in the process, the part of the dynamical equation that is due to surface diffusion would thereby obey a continuity equation

$$\frac{\partial h}{\partial t} \propto -\nabla \cdot J$$
 (2.27)

substituting for the current J we get,

$$\frac{\partial h}{\partial t} = -\sigma \nabla^2 (\nabla^2 h)$$

$$= -\sigma \nabla^4 h$$
(2.28)

#### 2.3.3 Linear Model with Surface Diffusion and Desorption

If both desorption and surface diffusion are present in the system, they must both be added to the dynamical equation describing the rate of change of the height.

$$\frac{\partial h}{\partial t} = -\sigma \nabla^2 (\nabla^2 h) + \nu \nabla^2 h + constant.$$
 (2.29)

Notice that all the microscopic details are hidden in the constants  $\nu$  and  $\sigma$ . The above approach is a phenomenological one in that it takes only the essential physics into account to describe the process. Equation.(2.29) is a good approximation when we don't have a beam of incoming particles. In the presence of a beam, the simplest

modification would be to add the beam fluctuations to the above equation resulting in,

$$\frac{\partial h}{\partial t} = -\sigma \nabla^2 (\nabla^2 h) + \nu \nabla^2 h + \eta(x, t)$$
(2.30)

where

$$< \eta(x,t) >= 0, \qquad (2.31)$$
  
$$< \eta(x,t)\eta(x',t') >\sim \delta(x-x')\delta(t-t')$$

This equation is a generalisation of a model considered by Edwards and Wilkinson (EW)(Edwards and Wilkinson, 1982) who treated the case  $\sigma = 0$ . Equation.(2.30) being linear, can be analyzed exactly.

Fourier transforming equation.(2.30),

$$h_q(t) = \eta_q(t) - a(q)h_q(t)$$
 (2.32)

where

$$a(q) = \nu q^2 + \sigma q^4 \tag{2.33}$$

We could analyze this transformed equation further by a change of variables namely,

$$\phi(t) = h_q(t)e^{a(q)t}$$

$$h_q(t) = \phi(t)e^{-a(q)t}$$
(2.34)

with this definition equation. (2.32) becomes

$$\dot{\phi}_q(t) = \eta_q(t) e^{a(q)t} \tag{2.35}$$

Integrating the above equation we have,

$$\phi_q(t) = \phi_q(0) + \int_0^t dt' \eta_q(t') e^{a_q t'}$$
(2.36)

The correlation function is therefore,

$$<\phi_{q}(t)\phi_{-q}(t')>=\int_{0}^{t'}dt'\int_{0}^{t}dt<\eta_{q}(t)\eta_{-q}(t')>e^{a_{q}(t+t')}$$

$$+.$$
(2.37)
Transforming back and using t' > t we have,

$$< h_q(t)h_{-q}(t') > \sim \frac{1}{\nu q^2 + \sigma q^4} e^{(\nu q^2 + \sigma q^4)|t' - t|}$$
 (2.38)

The equal time correlation function is,

$$< h_q(t)h_{-q}(t) > \sim \frac{1 - e^{-2(\nu q^3 + \sigma q^4)t}}{\nu q^2 + \sigma q^4}$$
 (2.39)

Taking the limit  $t \to \infty$  after inverting the Fourier transform results in,

$$<(h(x,t)-h(0,t))^{2}>\sim \ln l\sqrt{(\frac{\nu}{\sigma})}$$
 (2.40)

and in the limit  $l \to \infty$ , where l is a measure of the system size.

$$<(h(x,t)-h(x,0))^2>\sim \frac{1}{\nu}\ln(\frac{\nu^2 t}{\sigma})$$
 (2.41)

In the limit of  $\sigma \rightarrow 0$  we recover the results of EW namely,

$$<(h(x,t)-h(0,t))^2>\sim l^{-(\frac{3-d}{3})}$$
 (2.42)

In the  $t \to \infty$  limit implying that  $\alpha = \frac{3-d}{2}$  and for  $l \to \infty$ , we get  $\beta = \frac{3-d}{4}$ . On the other hand, when  $\nu = 0$ ,  $\alpha = \frac{5-d}{2}$ . These results are consistent with the fact that growing interfaces evolve into rough surfaces. We shall next study these equations in the presence of non-linear terms.

### 2.3.4 The Kardar-Parisi-Zhang equation

The EW stochastic equation was generalized to include non-linearities by Kardar, Parisi and Zhang (KPZ) (Kardar, Parisi and Zhang, 1986; Medina et al., 1989)

$$\frac{\partial h}{\partial t} = \nu \nabla^2 h + \frac{\lambda}{2} (\nabla h)^2 + \eta(x, t), \qquad (2.43)$$

we have already studied the relevance of the linear terms in the above equation. The term that makes the equation non-linear is  $(\nabla h)^2$ . This term cannot be obtained from any Hamiltonian and has a kinetic origin. It can however be derived from a weak gradient expansion, as we shall see shortly. Assuming that growth takes place



Figure 2.4: A picture showing the increment in h as the local growth occurs normal to the interface. normal to the local interface. Using Fig. 2.4, the increment at a point on the interface due to the deposition of a particle , may be written as,

$$\delta h = [(v\delta t)^2 + (v\delta t\nabla h)^2]^{1/2}$$
(2.44)

If the gradients are small,

$$\frac{\partial h}{\partial t} \sim v + \frac{v}{2} (\nabla h)^2 + \dots \qquad (2.45)$$

where v is the velocity normal to the interface. If we transform the problem into a co-moving frame, the velocity term can be transformed away. The noise term is assumed to be Gaussian in nature and its correlations are defined as before. The KPZ equation is arrived at by putting all these ingredients together.

#### A pedestrian analysis of the KPZ equation

(a). The KPZ equation is invariant under translations  $h \rightarrow h + constant$ .

(b). The sign of the coefficient of the driving term i.e  $\lambda$  is irrelevant as it can be changed by the transformation  $h \rightarrow -h$  and  $\lambda \rightarrow -\lambda$  which leaves the equation invariant.

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(c). It can be shown that the critical dimension  $d_c$  of the model is 2+1, which implies that the non-linear term is important at least in dimensions  $d \le 2+1$ . Dividing the non-linear term by the linear term we get,

$$\frac{(\nabla h)^2}{\nabla^2 h} \sim l \tag{2.46}$$

The above ratio diverges for large *l*. The argument also suggests that the non-linear term is more relevant when compared to the linear term.

(d). A power counting analysis shows that all higher order non-linear terms that may be added to the KPZ equation are irrelevant in the long wavelength limit and can thus be ignored.

(e). Considering the non-linear term alone in the absence of any thermal fluctuations, we can estimate the relaxation time of a mound of material on the surface, i.e

$$\frac{h}{\tau} \sim \lambda (\frac{h}{\zeta})^2 \tag{2.47}$$

$$\tau \sim \frac{\zeta^2}{\lambda h} \tag{2.48}$$

From the scaling properties of rough surfaces, we have  $h \sim \tau^{\beta}$  and  $\zeta \sim \tau^{\frac{1}{\beta}}$ . Using these relations in the above expression for the relaxation time  $\tau$ , one gets at a hyperscaling relation among the exponents,

$$\alpha + z = 2 \tag{2.49}$$

This scaling relation is true only when  $\lambda \neq 0$ . The above argument has been based on the non-trivial assumption that the coefficient  $\lambda$  is not renormalized by the noise. It can be shown as will be in the next chapter that this interesting property is intimately connected to the Galilean invariance of the KPZ equation. The exponents predicted by the KPZ equation are in excellent agreement those of the Eden model in 2 spatial dimensions, these two models are thus in the same universality class at least in d =1 + 1. Results in d = 2 + 1 are however uncertain as far as the KPZ equation goes, because this equation does not have a stable infrared fixed point as we shall see in

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the next chapter in dimensions  $d \ge 2 + 1$ .

(f). The KPZ equation can be mapped to two other useful equations. Using the Hopf-Cole transformation  $P(x,t) = e^{\frac{\lambda h(x,t)}{2\nu}}$  we obtain,

$$\frac{\partial P}{\partial t} = \nu \nabla^2 P + \left(\frac{\lambda}{2\nu}\right) \eta(x, t) P, \qquad (2.50)$$

which is a diffusion equation with a time-dependent random potential. The function P(x,t) may be regarded as a sum of Boltzmann weights of all the static configurations of a directed polymer(Huse, Henley and Fisher, 1985). A second transformation  $\vec{v} = -\nabla h$ , turns the equation into the randomly forced Burgers equation for a vorticity-free velocity field (Burgers, 1974),

$$\frac{\partial \vec{v}}{\partial t} + \lambda \vec{v} \cdot \nabla \vec{v} = \nu \nabla^2 \vec{v} + f(\mathbf{x}, \mathbf{t})$$
(2.51)

### 2.3.5 Growth equations without desorption

So far we have discussed the significance of desorption and its significance on the relaxation of a crystal through linear as well as non-linear equations. From the previous discussion it is clear that the KPZ equation neglects higher order terms as they don't play an important role in the long wavelength limit. The next question is : what happens at short wavelengths ?. To understand this, higher order terms would have to be included. The simplest thing would be to reintroduce the  $\sigma$  term. Let us start by turning off the  $\nu$  or desorption term. This leads to,

$$\frac{\partial h}{\partial t} = -\sigma \nabla^4 h + \eta(x, t), \qquad (2.52)$$

this equation being linear can be studied exactly as was done in the previous section. One could generalize the above equation to include non-linear terms too. A power counting analysis shows that non-linear terms proportional to  $\nabla^2 (\nabla h)^2$ ,  $(\nabla^2 h)^2$  and  $\nabla \cdot (\nabla h)^3$  are all relevant in dimensions  $d \leq 4 + 1$ . Thus in principle we could construct three different non-linear equations with each of these terms. One motivation behind studying an equation using surface diffusion as the sole relaxation term is the following: it is known that in the temperature range where MBE is normally



Figure 2.5: Diagram showing the direction of the flow of atoms on the surface.

conducted, relaxation occurs via rapid surface diffusion and that relaxation due to the desorption is negligibly small. Another important fact is that under ideal MBE growth conditions, it is thought that mass on the surface is conserved. In constructing a growth equation with a conserved quantity, the simplest way to accomplish it is to write down the following equation,

$$\frac{\partial h}{\partial t} = -\nabla \cdot J + \eta(x, t). \qquad (2.53)$$

Moreover, if the current J is considered to be made up of a linear and non-linear part, this puts restrictions on the type of non-linear term that may be chosen. The following equation was proposed by Lai and Das Sarma(Lai and Sarma, 1991) and Wolf and Villain(Wolf and Villain, 1990),

$$\frac{\partial h}{\partial t} = -\sigma \nabla^4 h + \lambda \nabla^2 (\nabla h)^2 + \eta(x, t), \qquad (2.54)$$

to account for MBE growth. We could get more insight about the physical process in question by considering the following. It has been experimentally observed that atoms landing at a kink on the surface prefer moving about on the same layer Fig. 2.5, rather than jumping onto a lower layer. This is because there is an effective potential barrier

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Figure 2.6: The potential interpretation of an interface step.

at the kink (Schwoebel, 1969; Roland and Gilmer, 1991; Fink and Erlich, 1986), see Fig. 2.6. One could approximate a kink by say,  $h \sim \tanh(x)$ . Fig. 2.7 shows a number of its derivatives. It is clear from this simple observation that sites near the bottom of a kink tend to grow more than the top and that sites with very steep gradients are not favourable for growth ruling out Fig. 2.7d as a possible non-linearity. Coming back to a discussion of terms in equation. (2.54), the surface diffusion term seems consistent with the facts. Regarding the non-linear term, Fig. 2.7c, it may be interpreted as the term that takes into account the atoms that break away from the kink sites at higher temperatures. The other possible non-linear term Fig. 2.7e seems to mimic the same physics but it is inconsistent with the demands of the continuity relation. We shall examine this equation in more detail in a later chapter. It turns out that all the exponents of equation. (2.54) may be evaluated using arguments à la Flory. As before we can estimate the relaxation time  $\tau$  of a mound of material of linear dimension *l* due to the above dynamics,

$$\tau \approx \frac{l^4}{\sigma + \nu h}.\tag{2.55}$$



Figure 2.7: A qualitative description of the local surface shape and its various derivatives.

One can also estimate the number of atoms n deposited in time  $\tau$ ,

$$n \approx l^{d-1} \frac{\tau}{\tau_o} \overline{F}.$$
 (2.56)

where  $\overline{F}$  is the fluctuation in the incoming beam of particles and  $\tau_o$  is the total time of deposition. It is the fluctuation in this number that causes the material to accrue into a mound. The fluctuation in the number is given by the square root of the above equation.(2.56). This quantity should also be equal to the number of particles deposited in a total time  $\tau$  i.e the total volume divided by the volume of an individual atom which can be taken to be unity. Therefore,

$$\tau \approx l^{d-1} \tau_o h^2. \tag{2.57}$$

h is the height of the deposit. Equating the above relations we have,

$$l^{d-1}\tau_o h^2 \approx \frac{l^4}{\sigma + \nu h}.$$
 (2.58)

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$$h^2(\sigma + \nu h) \approx l^{5-4}.$$
 (2.59)

This argument tells us that the coefficient  $\sigma$  does not influence the relaxation time for large lengthscales. From equation.(2.59) we clearly see that the width diverges for large linear dimensions l, in other words the surface is rough for dimensions  $d \leq 5$ . The exponent  $\alpha$  can be easily shown to be  $\frac{5-d}{3}$ . A simple substitution shows that  $z = \frac{7+d}{3}$ , resulting in the hyperscaling relation  $\alpha + z = 4$ . This relation can be shown to stem from a particular symmetry exhibited by equation.(2.54)(Sun, Guo and Grant, 1989). All the above exponents may be derived from a more rigourous renormalization group analysis (Lai and Sarma, 1991). Compared to the KPZ equation where the surface roughness increases due to the non-linear term, the roughness here seems to decrease.

### 2.3.6 Surface diffusion and shadowing

The microstructure associated with sputter deposition that we saw in the previous chapter is believed to be due to shadowing meaning that a particular site is entirely shadowed by the presence of very high 'mountains' of material near it, see Fig. 2.8 If the growth is by isotropic sputtering, then the growth rate of a site is approximately proportional to the exposure angle  $\theta$  of the site in question(Bruinsma, Karunasiri and Rudnick, 1990). This shadowing mechanism leads to unstable structures resulting in surface roughening. Thus the growth rate at a particular site is strongly influenced by the surface structure of nearby and not so nearby regions. This feature makes the problem non-local. If the incoming atoms are collimated into a beam in the normal direction see Fig. 2.8, this non-locality is not pronounced. This is the case with MBE, a deposition process we have already seen in the previous chapter. For a spread in incident angles, this effect is very strong and is the cause of the intricate microstructure we see in the case of sputter deposition.

The shadow model is thus based on the idea that global shadowing is the destabilising mechanism of growth in sputtering. The instabilities caused by shadowing are annealed to a certain extent by surface relaxation terms like surface diffusion and desorption. In this section we shall only focus on how shadowing competes with surface diffusion as this is the most dominant term at small lengthscales. As before



Figure 2.8: Diagrams showing the non-local shadowing effect and deposition by MBE.

we can write down our model for the rate of change of the height variable,

$$\frac{\partial h}{\partial t} = -\sigma \nabla^4 h + \gamma \theta + \eta(\theta), \qquad (2.60)$$

the first term as we very well know by now is due to surface diffusion, the second term is the shadowing term which takes into account all the incoming directions. The non-local nature of  $\theta$  makes the above model a formidable mathematical problem for analytic work. The problem can however be tackled numerically(Bales and Zangwill, 1989; Karunasiri, Bruinsma and Rudnick, 1989; Yao, Roland and Guo, 1992). Results from this analysis seem to show a columnar structure for the surface at late times, see Fig.(2.9). The shadowing problem has also been studied using the Monte Carlo approach(Roland and Guo, 1991) and results show a mountainous landscape. This Shadow model seems to provide us with a reasonable explanation for the microstructure observed in the sputtering process.

In this chapter we have reviewed models both numerical and phenomenological and have studied some simple ways of dealing with them like the Flory analysis. This argument that we used to analyze one of our equations cannot always be applied. The method infact breaks down in certain situations. In the next chapter we shall



Figure 2.9: Columnar landscape as a result of shadowing.

study a more rigourous method of approaching these non-linear problems namely the Renormalization Group analysis. We shall illustrate the method by applying it to the KPZ equation.

### Chapter 3

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## Interfaces and the Renormalization Group

### 3.1 Introduction

Having gotten ourselves acquainted with the general elements of static and dynamic interfaces in Chapters 1 and 2, we shall in this chapter study the renormalization group and how it could be used to analyze equilibrium and non-equilibrium interface problems. Before getting into the actual renormalization group method, we shall first review certain key concepts from critical phenomena which would be of use to us later. The term critical phenomena in simple language refers to the thermodynamic properties of a system near the critical temperature  $T_c$  of a second order phase transition. Typical examples of such a transition are the gas-liquid transition and the paramagnetic-ferromagnetic phase transition.

For an introductory review, we shall use the ferromagnetic system. As we all know, it is the unpaired electrons that are responsible for the magnetization of a material. In terms of energy, these electrons prefer aligning themselves in the same direction to lower the net energy due to the spin exchange interaction, which is caused as a result of the combined effect of the Coulomb interaction and the Pauli exclusion principle. When we lower the temperature to T = 0, all spins tend to align themselves and in this configuration, the system has a net magnetization and is said to have a ferromagnetic property. As one raises the temperature to finite T, the spins get randomised and the magnetization is reduced. Increasing the temperature further drastically reduces the spins aligned and at  $T = T_c$  this magnetization falls to zero and one has a paramagnetic material. In other words for  $T < T_c$ , order dominates, while for  $T > T_c$  disorder has the upper hand. Around  $T \sim T_c$ , there are large regions of aligned and misaligned spins. When these regions become large, the time required for ordering and disordering becomes proportionately long. As a result, spins are flipped around at random without any spatial or temporal coherence.

Critical phenomena may be classified as static or dynamic depending on whether one is dealing with equilibrium or the approach to equilibrium properties of a system. Statics normally deal with quantities like the specific heat, susceptibility, magnetization, etc and dynamics with the relaxation times, diffusion etc.

It has been observed experimentally that at temperatures very close to  $T_c$  quantities such as the magnetization, susceptibility, specific heat, etc go as powers of the temperature. These powers to which the temperature is raised are called critical exponents. These exponents help describe the nature of the singularities in various measurable quantities at the critical point. Defining a reduced temperature  $t = \frac{T - T_c}{T_c}$ . In the limit  $t \rightarrow 0$  any thermodynamic quantity can be decomposed into a regular part which remains finite and a singular part that may be divergent or have divergent derivatives. It is this singular part that is assumed to be proportional to some power(generally fractional) of the reduced temperature for example, the heat capacity  $C \sim |t|^{-\alpha}$ , the susceptibility  $\chi \sim |t|^{-\gamma}$ , etc. The significance of these critical exponents lie in their universality. A large number of experiments have shown that widely different systems exhibit the same critical exponents, these systems are said to belong to the same universality class, a magnet for example may have the same critical exponents as a gaseous system near the critical point, in other words details such as atomic interactions become irrelevant near  $T_c$ . The only quantity of relevance being the correlation length which diverges at the transition temperature. Another interesting aspect of these exponents is the fact that they exhibit scaling laws that are universal.

### 3.1.1 Scaling

Scaling as the name implies tells us how physical quantities change with respect to length scales. All one has to do is express the dimension of the quantity in question in terms of a standard unit of length, scaling then tells us how this quantity varies. Thus, a dimensionless quantity will be invariant in this scheme. A large number of important scaling laws may be derived for various thermodynamic functions around the critical temperature  $T_c$  by making the assumption that the correlation length is the only characteristic length of the system in terms of which all other lengths must be measured. Scaling when combined with the experimental fact that the correlation length  $\xi$  diverges at  $T \sim T_c$  leads to the conclusion that the system is invariant under scale transformations and that it has no characteristic length. Thus the system looks alike at all length scales. We shall soon see that this idea actually forms the basis upon which the whole concept of renormalization rests.

### **3.1.2** The Renormalization Scheme

In physics it is fairly easy to find systems that have many degrees of freedom in a region the size of a correlation length, critical phenomena is no exception. These systems behave differently when compared to systems that have a few degrees of freedom in one correlation length. Ordinarily one may describe a system completely using an interaction Hamiltonian, which encompasses within it all the necessary interactions. This is however true only when the correlation length is small. In critical phenomena however, degrees of freedom tend to interact with eachother giving rise to the collective behaviour we observe. The interaction Hamiltonian becomes a secondary object in this case. These systems become fairly difficult to handle precisely due to these interactions among the degrees of freedom. Renormalization provides us with a way I

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to handle these interactions. This approach may be summarized in two steps(Wilson and Kogut, 1974; Wilson, 1971),

(a). averaging out fast oscillations, in other words oscillations that are of length scales far smaller than the correlation length near the critical point, thereby reducing the degrees of freedom.

(b). helps account for the cooperative behaviour among the degrees of freedom.

The above steps are achieved by subjecting the system to a group of transformations that are in general linear (but maybe non-linear in certain cases), the effective number of the degrees of freedom are reduced in a step wise manner. These transformations are applied repeatedly till the spacing between the reduced degrees of freedom is roughly of order correlation length. The system is said to have reached a 'fixed point' at this stage, any further transformation at this point would yield the same results, the system in other words cannot be rescaled anymore. In the next and subsequent section, we shall see how this technique may be used to analyze interfaces both static and dynamic.

### 3.2 Renormalization as applied to static interfaces

In this section we shall briefly review some ways effective interface Hamiltonians may be studied using the renormalization scheme. As discussed in chapter 1, interfacial configurations may be described using a single-valued variable  $\phi(x, t)$ . The Hamiltonian then has the general form,

$$H(\phi) = H_o(\phi) + H_i(\phi) \tag{3.1}$$

where  $H_o(\phi)$  is the free part of the Hamiltonian and  $H_1(\phi)$  is the part that has all the interactions built into it and in general could be some potential V(x). As before the renormalization scheme may be broken down into a few crucial steps, we shall deal with each one of them in brief. First, the fluctuating interface function  $\phi(x)$  is broken down into fast and slow varying parts,

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$$\phi(x) = \phi_{<}(x) + \phi_{>}(x),$$
 (3.2)

This decomposition of the fast and slow modes is done in such a way that the free part of the Hamiltonian  $H_o(\phi)$  also decomposes into a fast and slow part(Wilson, 1971; Wilson and Kogut, 1974; Fisher and Huse, 1986; Halpin-Healy, 1989; Jasnow, 1986; Forgacs, Lipowsky and Nieuwenhuizen, 1991).

$$H_o(\phi) = H_o(\phi_{<}) + H_o(\phi_{>}).$$
 (3.3)

The next step involves integrating out the fast variables or fluctuations of the fluctuating function  $\phi(x)$ . The integration of the fast variables gives rise to an effective Hamiltonian  $H'(\phi_{<})$  for the slow oscillations. From the above equations we can then write,

$$H(\phi_{>} + \phi_{<}) = H_{o}(\phi_{<}) + H_{o}(\phi_{>}) + H_{i}(\phi_{>} + \phi_{<})$$
(3.4)

The averaging over the fast fluctuations is usually done using a suitable weight function (normally corresponding to the free interface Hamiltonian or Harmonic weight). The new effective Hamiltonian generated as a result of the averaging may not preserve the form of the original one. The averaging procedure introduces extra terms and one would have to deal with them or give physical arguments for their irrelevance. In general, the above procedure may not be an easy one technically, the degree of difficulty depending directly on the type of potential in use. The final step involves the rescaling of the spatial coordinates by a suitable factor in an effort to bring the problem back to its original form. This procedure is carried out again and again till one reaches a condition when the terms no longer renormalize i.e, application of the transformation generates the same terms as the previous step. The potential at this stage is said to be renormalized.

### **3.3 Dynamical Renormalization**

### 3.3.1 Introduction

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The effective interface Hamiltonians that we considered in the introductory chapter are insufficient when it comes to describing the dynamics. In this case one has to specify an equation of motion for the order parameter for example, say  $\phi(x, t)$ . The equation of motion describing the dynamics of this quantity is then simply given by the time dependent Ginzburg-Landau equation(TDGL),

$$\frac{\partial \phi(x,t)}{\partial t} = -D \frac{\delta H}{\delta \phi} + \eta(x,t), \qquad (3.5)$$

where  $H(\phi)$  is the Hamiltonian describing the static properties of  $\phi(x, t)$  and  $\eta(x, t)$ is the thermal noise in the system which is assumed to be Gaussianly distributed. As we can clearly see, equation.(3.5) is basically a Langevin equation. Depending on whether the order parameter is conserved or non-conserved, equations of the above type may be classified into model B or model A(Hohenberg and Halperin, 1977). A renormalization analysis on the above equation yields both the static and dynamic properties of the system. Other than technical differences, the renormalization analysis in dynamics is basically the same as in statics. Two widely used formalisms are, (a). the lagrangian formulation of Martin-Siggia-Rose (MSR)(Martin, Siggia and Rose, 1973; Bausch, Janssen and Wagner, 1976; Amit, 1984) which allows one to calculate all the dynamic correlations using rigorous methods from field theory,

(b). the momentum-shell renormalization of Ma, which essentially helps 'peel' off the fast modes in a systematic manner (Ma, 1980; Ma and Mazenko, 1975).

The above dynamical formulation is directly related to the fact that one can find a Hamiltonian that describes the static properties of the system. It is therefore limited to explaining critical dynamics, near equilibrium. We shall in the next section review a formulation due to Forster, Nelson and Stephen(Forster, Nelson and Stephen, 1977), that would enable us analyze systems that are far away from equilibrium such as the KPZ equation and other related ones.

# 3.3.2 Momentum-shell renormalization group analysis of the KPZ equation

A variant of the momentum-shell renormalization technique of Ma was used by Forster, Nelson and Stephen(Forster, Nelson and Stephen, 1977) in their analysis of the randomly forced Burgers equation which as we may recall from chapter 2 can be mapped to the KPZ equation by a simple transformation(Kardar, Parisi and Zhang, 1986; Medina *et al.*, 1989). It has been shown by Kardar et al that their analysis was valid for the KPZ equation as well. The momentum-shell method they used basically comprised two main steps:

- (a). integrating out the large k's
- (b). rescaling the remaining k's to restore the original k-space

We shall now sketch the method of Kardar et al. Starting with the KPZ equation,

$$\frac{\partial h}{\partial t} = \nu \nabla^2 h + \frac{\lambda}{2} (\nabla h)^2 + \eta(x, t), \qquad (3.6)$$

We first Fourier transform the above equation, using the following definitions of the transform and its inverse.

$$h(\vec{k},\omega) = \int d^{d-1}x \int_{-\infty}^{+\infty} dt h(\vec{x},t) e^{-\imath \vec{k} \cdot \vec{x} + \imath \omega t},$$
  
$$\eta(\vec{k},\omega) = \int d^{d-1}x \int_{-\infty}^{+\infty} dt \eta(\vec{x},t) e^{-\imath \vec{k} \cdot \vec{x} + \imath \omega t}.$$
(3.7)

where  $\Lambda$  is a lower cut-off on the wavelength, as one cannot probe lengths shorter than the lattice constant.

The inverse may be defined as

$$h(\vec{x},t) = \int_{k<\Lambda} \frac{d^{d-1}k}{(2\pi)^{d-1}} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} h(\vec{k},\omega) e^{i\vec{k}\cdot\vec{x}+i\omega t},$$
$$\eta(\vec{x},t) = \int_{k<\Lambda} \frac{d^{d-1}k}{(2\pi)^{d-1}} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \eta(\vec{k},\omega) e^{i\vec{k}\cdot\vec{x}+i\omega t}.$$
(3.8)

Substituting these definitions into the KPZ equation we get,

$$h(\vec{k},\omega) = h^{o}(\vec{k},\omega) - \frac{\lambda}{2}G_{o}(\vec{k},\omega) \int_{q,\Omega} \vec{q} \cdot (\vec{k}-\vec{q})h(\vec{q},\Omega)h(\vec{k}-\vec{q},\omega-\Omega), \qquad (3.9)$$



Figure 3.1: Diagrammatic representation of equation.(3.9).

$$<\eta(ec{k},\omega)>=0,$$

$$<\eta(\vec{k},\omega\eta(\vec{k}',\omega'))>=2D(2\pi)^d\delta(\vec{k}+\vec{k}')\delta(\omega+\omega')$$
(3.10)

The bare propagator or Green's function is given by,

$$G_o(\vec{k},\omega) = -\frac{1}{-i\omega + \nu k^2},$$
  
$$h^o(\vec{k},\omega) = G_o(\vec{k},\omega)\eta(\vec{k},\omega).$$
(3.11)

We next decompose all the fluctuations in the problem as fast and slow before carrying out the integration over all the fastmodes. All the averages are performed over the stochastic noise defined by equation.( 3.10). The correction to the response function  $G(\vec{k}, \omega)$  to lowest order in perturbation theory can then be shown to be, see Fig. 3.1,

$$G(\vec{k},\omega) = G_o(\vec{k},\omega) + 4(\frac{-\lambda}{2})^2 G_o^2(\vec{k},\omega)$$

$$\times \int_{q,\Omega} \frac{1}{(2\pi)^d} \vec{q} \cdot (\vec{k}-\vec{q}) \vec{q} \cdot \vec{k} G_o(\vec{k}-\vec{q},\omega-\Omega) G_o(\vec{q},\Omega) G_o(-\vec{q},-\Omega) 2D(\vec{q},\Omega)$$

$$+ O(\lambda^4), \quad (3.12)$$

the factor of four stemming from the various possible noise contractions. Fig. 3.2 diagrammatically represents the above lowest-order (one-loop) correction to the response function, the noise spectral density function and the effective vertex function.

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Figure 3.2: (a) the response function, (b) the noise spectral density function, (c) the vertex function.

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#### INTERFACES AND THE RENORMALIZATION GROUP

To first order the surface tension  $\nu$  then renormalizes as,

$$\nu_r = \nu \left[1 + \frac{\overline{\lambda}^2 K_{d-1}}{4(d-1)} \left(e^{-l(d-3)} - 1\right)\right]$$
(3.13)

Similarly we have,

$$D_r = D[1 - \frac{\overline{\lambda}^2 K_{d-1}}{4(d-3)} (e^{-i(d-3)} - 1)]$$
(3.14)

The coupling constant  $\lambda$  does not renormalize due to Galilean invariance (Kardar, Parisi and Zhang, 1986). Therefore,

$$\lambda_r = \lambda \tag{3.15}$$

In the above equations  $K_{d-1} = \frac{1}{2^{d-2}\pi^{\frac{d-1}{2}}}\Gamma(\frac{d-1}{2})$  is a constant of integration corresponding to a (d-1) dimensional surface and  $\overline{\lambda}^2 = \frac{\lambda^3 D}{\nu^3}$ . Having integrated away the large k's, we must now rescale our coordinates to restore the original k space. We therefore perform the following transformations,

$$\vec{k}' = e'\vec{k},$$

$$\omega'=e^{*\prime}\omega,$$

To ensure that the height variable h still satisfies the KPZ equation we perform the following rescalings which ensure this,

$$h'(\vec{k}',\omega') = e^{-2l - (d + \alpha - 1)l} h(\vec{k},\omega),$$
  
$$\eta'(\vec{k}',\omega') = e^{-(d + \alpha - 1)l} \eta(\vec{k},\omega).$$
 (3.16)

Using these expressions we obtain,

$$\nu(l)=e^{(z-2)l}\nu_r,$$

$$D(l) = e^{(z-2\alpha-d+1)l}D_{\tau}$$

$$\lambda(l) = e^{(z-2+\alpha)l} \lambda_r. \tag{3.17}$$

Treating l as infinitesimal one gets the following recursion relations,

$$\frac{d\nu(l)}{dl} = \nu(l)[z - 2 + \frac{\overline{\lambda}^2 K_{d-1} \frac{3 - d}{d - 1}]$$
(3.18)

$$\frac{dD(l)}{dl} = D(l)[z - d + 1 - 2\alpha + \frac{\overline{\lambda}^2 K_{d-1}}{4}]$$
(3.19)

$$\frac{d\lambda(l)}{dl} = \lambda(l)[z - 2 + \alpha]$$
(3.20)

The flow equation for the effective coupling constant  $\overline{\lambda}$  is therefore,

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$$\frac{d\overline{\lambda}(l)}{dl} = \frac{3-d}{2}\overline{\lambda} + K_{d-1}\frac{2d-5}{4d-4}\overline{\lambda}^3.$$
(3.21)

to leading order in  $\overline{\lambda}$ . It can be shown that the 'critical dimension'  $d_c = 2 + 1$  for the KPZ equation which implies that for  $d \ge 2 + 1$ , the non-linear term in the equation becomes irrelevant and one should get back linear results. At d = 2 + 1 however, the strong coupling fixed point cannot be probed using the perturbation theory because the  $\overline{\lambda}^3$  term in equation.(3.21) remains positive always, making the equation diverge for large  $\overline{\lambda}$ . There however exists a strong coupling fixed point in d = 1 + 1, at this fixed point setting the recursion relations (equations.(3.18),(3.19) and (3.20)) to zero, one gets the exponents  $\beta = \frac{1}{3}$ ,  $\alpha = \frac{1}{2}$  and  $z = \frac{3}{2}$  which agree very well with numerical simulations on the Eden model. There has however, been much work on the numerical side in d = 2 + 1(Guo, Grossmann and Grant, 1990a; Armar and Family, 1990; Kim and Kosterlitz, 1989; Guo, Grossmann and Grant, 1990b) using both Langevin and Monte Carlo simulations.

### Chapter 4

## Numerical Study of a Model for Driven Interface Dynamics

In this chapter we shall study the consequence of adding the non-linear term corresponding to Fig. (2.7e), i.e  $(\nabla^2 h)^2$  to the following linear equation governed by surface diffusion.

$$\frac{\partial h}{\partial t} = -\sigma \nabla^4 h + \eta(x, t), \qquad (4.1)$$

The equation as a result becomes,

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$$\frac{\partial h}{\partial t} = -\sigma \nabla^4 h + \lambda (\nabla^2 h)^2 + \eta(x, t), \qquad (4.2)$$

This model differs from the non-linear model of Lai-DasSarma-Villain in the type of non-linearity used. It is clear eventhough the above equation cannot be written in the form of a continuity current, the non-linearity nevertheless helps mimic accrual of atoms at a kink thereby making equation.(4.2) a likely candidate to describe a non-linear growth process dictated by surface diffusion, the MBE growth process for example.

It turns out that if one considers linear equation.(4.1) as an expansion on the local curvature of the interface  $(K \sim \nabla^2 h)$ . Then equation.(4.1) gives a local growth rate,

$$v \sim -\sigma \nabla^2 K \tag{4.3}$$

Using the above equation as an expansion as already mentioned, if we expand up to the simplest non-linearity in K we get,

$$v \sim -\sigma \nabla^2 K + \lambda K^2 + \dots \tag{4.4}$$

The extra piece is essentially the same non-linear term as in Fig.(2.7e). This growth rate is very similar to that of the well known local model for dendritic growth (Kessler, Koplik and Levine, 1988; Pelce, 1988) which assumes that the local growth rate may be written as,

$$v \sim \nu K - \sigma \nabla^2 K + \lambda K^2 + \dots$$
(4.5)

The difference between the above two equations lies in the first term, this term combined with the second leads to the Mullins-Sekerka instability (Mullins and Sekerka, 1963; Mullins and Sekerka, 1964) which gives rise to the situation that lumps of material on the surface tend to grow faster. This equation has a band of unstable modes which can be shown by a linear stability analysis (Pelce, 1988). The  $K^2$  term is associated with the undercooling, which enhances the growth rate and also breaks the symmetry between the interior and exterior. Most of the work on the local model has been focussed on the steady state pattern that the equation generates. If one decides to study the dynamical scaling of such an interface, one may turn off the Mullins-Sekerka instability by making the assumption that the growth has already occured for a long time(Govind and Guo, 1992). The equation thus simplifies to,

$$v \sim -\sigma \nabla^2 K + \lambda K^2 + \dots \tag{4.6}$$

identical to equation.(4.2). Assuming that there are fluctuations in the system, the above equation can then be written as,

$$\frac{\partial h}{\partial t} = -\sigma \nabla^4 h + \lambda (\nabla^2 h)^2 + \eta(x, t).$$
(4.7)

This serves as a second motivation for studying equation.(4.2).

### 4.1 Renormalization Group analysis

We shall use the same renormalization scheme (the momentum-shell method) that was used to analyze the KPZ equation in chapter 3. Using the definitions of the transform and its inverse from chapter 3, we first Fourier transform equation.(4.2),

$$h(\vec{k},\omega) = h^{o}(\vec{k},\omega) + \frac{\lambda}{2}G_{o}(\vec{k},\omega)\int_{q,\Omega}\vec{q}^{e}(\vec{k}-\vec{q})^{2}h(\vec{q},\Omega)h(\vec{k}-\vec{q},\omega-\Omega), \qquad (4.8)$$

 $<\eta(ec{k},\omega)>=0,$ 

$$<\eta(\vec{k},\omega\eta(\vec{k}',\omega')) >= 2D(2\pi)^d \delta(\vec{k}+\vec{k}')\delta(\omega+\omega')$$
(4.9)

The bare propagator or Green's function is given by,

$$G_o(ec{k},\omega) = -rac{1}{-i\omega+\sigma k^4},$$

and

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$$h^{o}(\vec{k},\omega) = G_{o}(\vec{k},\omega)\eta(\vec{k},\omega).$$
(4.10)

The diagrammatic representation of the above expression is identical to Fig.(3.14). Infact all the diagrams that were used to renormalize the various constants in the KPZ equation may be used here as well. The fluctuations in the problem are then decomposed as fast and slow before the fast modes are integrated out. All the averages are performed over the stochastic noise defined by equation.(4.9). The correction to the response function  $G(\vec{k},\omega)$  to lowest order in perturbation theory can then be shown to be, see Fig.(3.1),

$$G(\vec{k},\omega) = G_o(\vec{k},\omega) + 4(\frac{\lambda}{2})^2 G_o^2(\vec{k},\omega)$$

$$\times \int_{q,\Omega} \frac{1}{(2\pi)^d} \vec{q}^2 (\vec{k} - \vec{q})^2 \vec{q}^2 \vec{k}^2 G_o(\vec{k} - \vec{q},\omega - \Omega) G_o(\vec{q},\Omega) G_o(-\vec{q},-\Omega) 2D(\vec{q},\Omega)$$

$$+ O(\lambda^4), \quad (4.11)$$

the factor of four stemming from the various combinations of the noise contractions. The diagrams being exactly identical to the ones used to analyze the KPZ equation, it is relatively straight forward to show to first order that  $\sigma$  renormalizes as,

$$\sigma_r = \sigma \left[1 + \frac{\lambda^2 D K_{d-1} l}{4\sigma^3}\right] \tag{4.12}$$

Similarly we have,

$$D_{r} = D[1 + \frac{\lambda^{2} D K_{d-1}}{4\sigma^{3}}]$$
(4.13)

The coupling constant  $\lambda$  renormalizes in this case as there is no Galilean invariance in the problem. We found,

$$\lambda_r = \lambda \left[1 + \frac{\lambda^2 D K_{d-1} l}{4\sigma^3}\right] \tag{4.14}$$

In the above equations  $K_{d-1} = \frac{1}{2^{d-2}\pi^{\frac{d-1}{2}}}\Gamma(\frac{d-1}{2})$  is a constant of integration corresponding to a (d-1) dimensional surface. As before we restore the full k space using the following transformations,

$$\vec{k}' = e^{l}\vec{k},$$

$$\omega' = e^{zl}\omega,$$

$$h'(\vec{k}',\omega') = e^{-zl-(d+\alpha-1)l}h(\vec{k},\omega),$$

$$\eta'(\vec{k}',\omega') = e^{-(d+\alpha-1)l}\eta(\vec{k},\omega).$$
(4.15)

Using these expressions we obtain,

$$\sigma(l) = e^{(z-4)l}\sigma_r,$$

$$D(l) = e^{(z-2\alpha-d+1)l}D_r,$$

$$\lambda(l) = e^{(z-2+\alpha)l}\lambda_r.$$
(4.16)

#### NUMERICAL STUDY OF A MODEL....

Treating *l* as infinitesimal one gets the following recursion relations,

$$\frac{d\sigma(l)}{dl} = \sigma(l)[z-4+\frac{\overline{\lambda}^2 K_{d-1}}{4}]$$
(4.17)

$$\frac{dD(l)}{dl} = D(l)[z - d + 1 - 2\alpha + \frac{\overline{\lambda}^2 K_{d-1}}{4}]$$
(4.18)

$$\frac{d\lambda(l)}{dl} = \lambda(l)[z - 4 + \alpha + \frac{\overline{\lambda}^2 K_{d-1}}{4}]$$
(4.19)

where  $\overline{\lambda}^2 = \frac{\lambda^3 D}{\nu^3}$ . The flow equation for the effective coupling constant  $\overline{\lambda}$  is then given by,

$$\frac{d\overline{\lambda}(l)}{dl} = \frac{5-d}{2}\overline{\lambda} + K_{d-1}\frac{3}{4}\overline{\lambda}^3.$$
(4.20)

to leading order in  $\overline{\lambda}$ . From the above equation we clearly see that above the critical dimension  $d_c = 4 + 1$ , one gets a stable fixed point at  $\overline{\lambda} = 0$  and the result z = 4 is obtained. However, below the critical dimension, no stable non-trivial fixed point can be found. There is also no simple hyperscaling relation between the exponents z and  $\alpha$ . A similar situation exists in d = 2 + 1 for the KPZ equation. The first order perturbative calculation in this case therefore does not allow us to probe a strong coupling fixed point in any physically relevant dimension.

The above calculation was also carried out using correlated noise whereby the noise correlations become,

$$<\eta(\vec{k},\omega)\eta(\vec{k}',\omega')=2D_{\rho}k^{-2\rho}\delta^{d-1}(\vec{k}+\vec{k}')\delta(\omega+\omega'), \qquad (4.21)$$

The calculation being identical to the uncorrelated case, one obtains the following recursion relations that depend on the noise exponent  $\rho$ ,

$$\frac{d\sigma(l)}{dl} = \sigma(l)[z-4+\frac{\overline{\lambda}^2 K_{d-1}}{4}], \qquad (4.22)$$

$$\frac{dD(l)}{dl} = D(l)[z - d + 1 - 2\alpha + 2\rho], \qquad (4.23)$$

and

$$\frac{d\lambda(l)}{dl} = \lambda(l)[z - 4 + \alpha + \overline{\lambda}^2 K_{d-1}].$$
(4.24)

Notice that the recursion relation for D results solely from scaling arguments implying that the correlated noise doesn't renormalize it as it does in the uncorrelated case. Further the the effective coupling constant  $\overline{\lambda}$  renormalizes as,

$$\frac{d\overline{\lambda}(l)}{dl} = \frac{5-d+2\rho}{2}\overline{\lambda} + K_{d-1}\frac{5}{8}\overline{\lambda}^3.$$
(4.25)

Thus we see that the spatially correlated noise changes the critical dimension of the model (the critical dimension being a function of  $\rho$  in this case). Unfortunately the coefficient of the  $\overline{\lambda}^3$  term still remains positive which prevents the model from having a stable fixed point.

### 4.2 Numerical analysis

Since the RG analysis did not lead to a strong coupling stable fixed point, a numerical integration of the problem was resorted to (Govind and Guo, 1992). The integration method that was used was the central finite difference and the Euler method. This method is perhaps the simplest numerical algorithm used widely over the years to solve differential equations. It consists in approximating the temporal and spatial derivatives as (Abramowitz and Stegun, 1975),

$$\frac{\partial h(x,t)}{\partial t} = \frac{h(x,t+\Delta t) - h(x,t-\Delta t)}{2\Delta t},$$
(4.26)

and

$$\frac{\partial h(x,t)}{\partial x} = \frac{h(x+\Delta x,t) - h(x-\Delta x,t)}{2\Delta x}.$$
(4.27)

Making use of these relations, equation.(4.2) may be written as,

$$h(x, t + \Delta t) = h(x, t) + \Delta t[(-\sigma) \frac{h(x + 2\Delta x, t) - 4h(x + \Delta x, t) + 6h(x, t) - 4h(x - \Delta x, t) + h(x - 2\Delta x, t)}{(\Delta x)^4} + (\frac{\lambda}{2})(\frac{h(x + \Delta x, t) - 2h(x, t) + h(x - \Delta x, t)}{(\Delta x)^2})^2 + \eta(x, t)]$$
(4.28)

#### NUMERICAL STUDY OF A MODEL....

There are however certain conditions that the Euler method must satisfy for its stability. Typically the values of  $\Delta x$ , and  $\Delta t$  must be chosen such that

$$\Delta x \ll L, \tag{4.29}$$

and

$$\Delta t \ll t \tag{4.30}$$

where L and t are the length and time scales associated with the problem. Since these quantities are not totally independent of eachother,  $\Delta x$  and  $\Delta t$  cannot be chosen arbitrarily and care must be taken in choosing them in such a way that numerical instabilities are avoided. The noise term  $\eta(x,t)$  was simulated using a suitable Gaussian random number generator which was tested to avoid any possible correlations among the numbers generated. In our simulations we used  $\Delta x = 1$  and  $\Delta t = 0.01$ . A small  $\Delta x$  implies that more points are taken into account. We have checked that a smaller time step does not change the results in any important manner. To obtain reasonable statistics, all the averages were performed over 100 independent runs.

### 4.2.1 Results in two spatial dimensions

We now report results from our simulations in d = 1 + 1 dimensions. The equation was solved using L = 512,  $\Delta t = 0.01$ ,  $\Delta x = 1$  for values of  $\lambda$  between 10 and 50. Fig.(4.1) shows a log-log plot between the width and the time. The slope of the straight line gives the value of  $\beta$ . For the largest 2 values of  $\lambda$ ,  $\beta$  was found to be  $0.39 \pm 0.03$ . The roughening exponent  $\alpha$  was obtained by integrating the equation till a steady state was reached for different values of system size L (see Fig.(4.2)). The slope of the line yields a value of  $\alpha = 1.4$ .

### 4.2.2 **Results in three spatial dimensions**

The equation was also integrated in the physically relevant d = 2+1 dimensions, using exactly the same values for  $\Delta x$  and  $\Delta t$  as in the d = 1+1 case. The width W as a ž

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Figure 4.1: The interface width W as a function of time t in d = 1 + 1. Each curve corresponds to an average of 100 independent runs on a system of size L = 512. Lower to higher curves correspond to  $\lambda = 10, 25, 40, 50$  respectively. The slope for the largest 2 values of  $\lambda$  give  $\beta = 0.39$ .



Figure 4.2: A log-log plot of the width W vs L at very large times. The slope gives a value of  $\alpha = 1.4$ .



Figure 4.3: The interface width W as a function of time t in d = 2 + 1. Each curve corresponds to an average of 100 independent runs on a system of size L = 50. The curves correspond to  $\lambda = 30, 50$  respectively. The slope yields a value  $\beta = 0.22$ .

function of time t was studied using values of  $\lambda = 30,50$  respectively (see Fig.(4.3)). The value of  $\beta$  was found to be 0.22 for both the curves shown in the figure.  $\beta$  was also determined using the two point correlation function  $G(t) = \langle (h(x,t+T) \cdot h(x,t))^2 \rangle$ , since  $G(t) \sim t^{2\beta}$  at intermediate times and was found to be  $0.21 \pm 0.02$  consistent to within error bars. The roughening exponent was determined in exactly the same way as in the d = 1 + 1 case, Fig.(4.4) shows a plot of the width W as a function of the system size L. We obtained a value of  $\alpha = 0.82 \pm 0.03$ . Fig.(4.5) shows a profile of the interface generated after a time t = 1000. This is to be compared with the interface shown in Fig.(4.6) which corresponds to the KPZ equation.

### 4.3 Summary and Discussion

In this chapter, we have proposed and studied a physically meaningful model relevant in describing kinetic roughening phenomena in the hydrodynamic limit of a growing interface where surface relaxation is controlled by surface diffusion. The model may be relevant in describing the roughening of the tip of a large dendrite(Maurer *et al.*,



Figure 4.4: A log-log plot of the width W vs L at very large times. The slope gives a value of  $\alpha = 0.82$ .



Figure 4.5: Typical shape of a surface generated by the model we investigated in this chapter after t = 1000.

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Figure 4.6: Typical shape of a surface generated by the KPZ model after t = 1000.



Figure 4.7: Picture showing the roughening of the tip of a large dendrite (Maurer et al, 1989).

1989) (see Fig. (4.7)). We see that the presence of the non-linear term reduces the value of the exponent  $\alpha$  when compared to the linear theory ( $\alpha = 1.5$ ), but is still higher than the  $\alpha = 1$  in d = 1 + 1. The width  $\frac{W(L,t\to\infty)}{L} \sim L^{\alpha-1}$  diverges for large L as a result, indicating a breakdown of the SOS condition discussed in an earlier chapter. This feature exists in other models as well where relaxation is controlled by surface diffusion. In d = 2 + 1 dimensions however,  $\alpha$  is reduced from the linear result of  $\alpha = 1$  to a smaller value due to the non-linear term. This  $\alpha$  is still quite large implying that surfaces generated as a result of the dynamics dictated by these equations are extremely rough. These equations are therefore insufficient in trying to account for growth by MBE which as we have already discussed helps generate surfaces that are extremely smooth. One therefore has to modify these equations suitably. A different non-linearity may be used, it however turns out that all other non-linear terms other than those disussed are irrelevant. Another possibility would be to include a conserved noise (Sun, Guo and Grant, 1989), which could arise from the extreme accurate collimation of the beam used to deposit atoms on the substrate. One could think of other possibilities too such as using a multiplicative noise. These status of research in this area is still very preliminary and further analysis needs to be done. It would be interesting to see how these continuum equations have to be modified in order that one gets exponents closer to reality. Further from the profiles of the interfaces in d = 2 + 1 shown in Figs. (4.5) and (4.6), it is clear that surface diffusion is not a very efficient mechanism in smoothing out large wavelength fluctuations whereas relaxation due to surface desorption is better at smoothing out these undulations. However, the surface in the former case is much smoother on smaller length scales compared to the latter. In conclusion we note that models with surface diffusion and non-conserved noise seem to give rather large roughening exponent values. It will be interesting to see what other effects can help alter the above situation.

### Chapter 5

## The Effects of Impurities on Driven Interfaces

The previous four chapters were devoted to the general understanding of interface dynamics, through continuum and lattice models. We must remember that those were only models and one can establish their validity only by comparing their predictions with experimental results. To date very few experiments have actually been performed to study kinetic roughening phenomena. This may be attributed to a number of factors, foremost among them being technical difficulty. There have nevertheless been some measurements on fluid flow through porous media (Rubbio et al., 1989; Rubbio et al., 1990; Martys, Cieplak and Robbins, ; Horvath, Family and Vicsek, 1991; Buldyrev et al., 1992) which have revealed roughening exponents that are vastly different from those predicted by theoretical models (Kardar, Parisi and Zhang, 1986; Kim and Kosterlitz, 1989). It is obvious that the standard models haven't taken something essential into account. The missing ingredient has to be the effect of quenched impurities, the random pore sizes that tend to pin the advancing fluid front, causing it to roughen further. Indeed, the experimentally measured roughening exponent  $\alpha$  is much larger than the theoretically predicted value. Therefore in constructing meaningful models this aspect has to be taken care of. In this chapter we shall review various models, lattice and continuum that take this into account and

we shall conclude with a discussion of our findings of the effect of quenched impurities on the driven dynamics of an interface with a conservation law.

### 5.1 Review of models with quenched noise

As we have already seen in the introductory chapter, a quenched random impurity may be modelled theoretically using random fields and bonds (Grinstein and Ma, 1982; Villain, 1982; Kardar, 1985) whereby one writes down an interface Hamiltonian with a random potential V. This gives us information about the static properties. For dynamic properties as already mentioned, we would have to start with a continuum equation. A simple way by which we may include these quenched impurities is by modifying the noise term. For example, consider a linear model,

$$\frac{\partial h}{\partial t} = \nu \nabla^2 h + \eta(x, h)$$
(5.1)

where the quenched noise correlations are given by,

$$\langle \eta(x,h)\eta(x',h')\rangle \sim \delta^d(x-x').$$
 (5.2)

The above model being linear can be analyzed exactly, it yields a  $\beta = 0.75$  compared to a  $\beta = 0.25$  if the noise were not quenched (refer chapter 2). This property is shared by other linear models as well. As far as a non-linear analysis goes there has been some recent work by Zhang and others(Zhang, 1990), who have tried to bridge the difference between theory and experiment by introducing a power law distributed instead of the more conventional Gaussian distributed noise into the KPZ equation. Zhang for example assumed the following distribution for for the noise  $\eta$ ,

$$P(\eta) \sim \frac{1}{\eta^{1+\nu}} \tag{5.3}$$

with  $\eta > 1$ . These authors have found noise dependent roughening exponents thus setting to nought all claims about the universality of these values. This discussion however leaves open the question as to what is the physical reason behind these non-universal exponents and the strange noise distribution given by equation.(5.3). In a recent paper Jensen and Procaccia(Jensen and Procaccia, 1991) have tried to answer this question using a generalised version of the Kim-Kosterlitz growth algorithm (Kim and Kosterlitz, 1989)(a model that corresponds to the lattice version of the KPZ equation) to include the effects of a quenched random background which would tend to pin the interface as it propagates forward. These authors found anomalous exponents consistent with the predictions of Zhang and others. The roughening exponent  $\alpha$  was found to be  $\approx 0.85$  far higher than the  $\approx 0.5$  obtained from the unmodified KK model proving that pinning does indeed roughen the interface further.

### 5.2 Effect of quenched impurities on the driven dynamics of an interface with a conservation law

In all the models studied so far, the interface advances through the random background potential. This almost never happens in solid systems. In this section we shall study the effects of a quenched impurity on a driven interface (thus non-equilibrium) which does not advance on average: the average position of the interface being fixed by a conservation law. Therefore, the interface although in non-equilibrium, can only fluctuate around its initial position. The interface being fixed (average position), thus experiences the same set of random impurities. We shall see later how one may take this feature into account. A realistic example is a surface being damaged by radiation with impurities trapped near the surface. The total number of atoms in the system is conserved but the system is far away from equilibrium. Before we get into the real discussion, we shall briefly review a few conserved models, lattice as well as continuum.
## 5.2.1 Models for Conserved Surface Dynamics

#### Continuum Model

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It is well known that the presence of a conservation law vastly changes the roughening dynamics of a system far from equilibrium. A well known model is one due to Sun, Guo and Grant(SGG)(Sun, Guo and Grant, 1989) in which the local growth rate of the interfacial height, h(x) is proportional to the divergence of a current. Therefore one has,

$$\frac{\partial h}{\partial t} = \nabla^2 \left[ -\nu \nabla^2 h + \frac{\lambda}{2} (\nabla h)^2 \right] + \eta(x, t), \qquad (5.4)$$

the noise-noise correlations being given by,

$$<\eta(x,t)\eta(x',t')>=-2D\nabla^2\delta^d(x-x')\delta(t-t')$$
(5.5)

and  $\nu$ ,  $\lambda$ , D are constants already defined in chapter 2. A dynamic renormalization group analysis on the above equation, yields scaling exponents  $\alpha = \frac{1}{3}$ ,  $\beta = \frac{1}{11}$  and  $z = \frac{11}{3}$ . These exponents also satisfy the scaling relation

$$\alpha + z = 4 \tag{5.6}$$

in all dimensions. These exponents being very different from those of the KPZ equation show that this model belongs to a different universality class. Since the growth rate is proportional to the divergence of a current, it is obvious that the total volume under the interface is always conserved. This model may correspond to the reconstruction of a laser damaged surface as mentioned above. The model being dominated by surface diffusion may also be relevant for the MBE growth process discussed in Chapters 2 and 4, there are reasons to expect this because of the small value of the  $\alpha$ (see above) generated by the model. This is another motivation to study a conserved model in the presence of quenched impurities.

### Lattice Model

Since the average position of the interface is fixed in time, it is quite tricky to formulate a lattice or microscopic model which must not only take care of this aspect but also break detailed balance in an appropriate manner so that the non-equilibrium nature of the model is preserved. Indeed such a lattice model was proposed by Racz et al(Racz et al., 1991) recently. Their model is basically a conserved variant of the restricted solid on solid model of Kim and Kosterlitz(Kim and Kosterlitz, 1989) and their algorithm goes as follows:

(a). Pick a site at random

(b). Increase its height by one and check if the height restriction is satisfied  $(|h(i) + \Delta - h(i \pm 1)| \le H)$ .

(c). If the above condition is not satisfied, go to step (1) and initiate the process again.

(d). If the condition is satisfied, this site is a potential site for an increase by the amount  $\Delta$ . The next thing is to find a suitable neighbour for a decrease so that local conservation is maintained. To do this, check both the nearest neighbours of the relevant site to see if any or both of them are capable of being decreased and at the same time keeping the height restriction condition of step (2) intact.

(e). If only one of the nearest neighbours is capable of being decreased, choose it and decrease its height by  $\Delta$ .

(f). If both are capable of being decreased, choose one at random and perform the decrease.

(h). If none can be found go back to step (1).

The conservation law is pretty obvious in the above set of rules. These growth rules can be shown to break detailed balance explicitly (Racz *et al.*, 1991) (see Fig.(5.1)). If  $P_a$ ,  $P_b$  and  $P_c$  are the steady state probabilities of states a, b and c and  $P_{ab}, P_{bc}$  and  $P_{ca}$ are the transition probabilities between these states, then detailed balance requires that,

$$P_a P_{ab} = P_b P_{ba}$$

$$P_a P_{ac} = P_c P_{ca}$$
(5.7)

which leads to the condition,

$$\frac{P_{ab}}{P_{ac}} = \frac{P_{ba}}{P_{ca}}.$$
(5.8)

where we have used the fact that  $P_b = P_c$  by periodic boundary conditions. However, from Fig.(5.1), we see that the right hand side of the above equation equals 1 whereas the left hand side equals  $\frac{1}{2}$  clearly showing the violation of detailed balance.

Studies on this model have shown that the ratio  $\frac{\Delta}{H}$  plays an important role in determining the universality class the model describes. At precisely  $\frac{\Delta}{H} = \frac{1}{3}$ , the model yields exponents consistent with the SGG model. For values greater and lesser than  $\frac{1}{3}$ , the model exhibits a smooth and grooved phase with exponents vastly different from those of the SGG model respectively (Racz *et al.*, 1991). One can indeed construct a rather interesting phase diagram corresponding to various values of this ratio.

## 5.2.2 Effect of quenched impurities

To study the effects of quenched impurities on a conserved system, we have generalised the above lattice model to take this into account (Govind, Guo and Grant, 1992). The impurities are represented by random pinning strengths on each lattice site (i, j). No site can be occupied or emptied until its pinning strength is reached. The pinning strengths are modeled by integer random numbers chosen between zero and some largest number  $M_{max}$  drawn from a uniform distribution, in other words each site (i, j) has a pinning strength  $0 \leq M_p(i, j) \leq M_{max}$ . Having defined the pinning indices, we now define two registers at each lattice site: a forward register  $R_f(i, j)$ and a backward register  $R_b(i, j)$ . The forward register  $R_f(i, j)$  keeps track of the number of occupying or growth attempts at a site and the backward register  $R_b(i, j)$ keeps track of the number of emptying attempts at a site. When an attempt is made to occupy a site, the forward register is increased by unity. Occupation of this site is permitted only if  $R_f(i, j) \geq M_p(i, j)$ . Similarly a decrease or emptying of a site is possible only if  $R_b(i, j) \geq M_p(i, j)$ . Of course, all increases or decreases are subjected to the height restriction condition already mentioned. Once all the heights



Figure 5.1: Transition probablities between various configurations showing the breaking of detailed balance i.e,  $\frac{P_{ab}}{P_{ba}} \neq \frac{P_{ac}}{P_{ca}}$  in the steady state

are updated, the registers are all re-set to zero. We have checked that we recover all the results of Racz et al if all the pinning strengths are the same throughout the lattice. This serves to check our code. However, when the pinning strengths are random, very different results are obtained.

All the simulations were done systems with 256 lattice sites. pinning tends to slow down the dynamics of the system, we ran the system proportionately longer for those simulations with high pinning values so that one deposits the same number of particles when compared to the zero pinning or no impurity case.

### **Results and Discussion**

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We now present our findings for simulations in 2 spatial dimensions. Since the model is very sensitive to the value of the  $\frac{\Delta}{H}$ , we first set this ratio to  $\frac{1}{3}$  which as we have already seen corresponds to the SGG model. The exponent  $\beta$  was calculated for various values of the pinning strengths. Fig.(5.2) shows many different curves corresponding to various values of pinning strengths. The plot of  $\beta$  vs the reciprocal of the maximum pinning strength  $M_{max}$  is however more informative (see Fig.(5.3)). As we can see,  $\beta$  seems to increase for increasing pinning strength but begins to saturate for very large pinning values. Notice that the exponents corresponding to the SGG model are retrieved when the pinning is very small. We have also determined the roughening or wandering exponent  $\alpha$  using the steady state structure factor S(k) defined by

$$S(k) = \frac{\langle h_i h_j e^{ik(i-j)} \rangle}{L}$$
(5.9)

where  $h_i$  and  $h_j$  are the heights at lattice sites i and j at very long times. The width W is related to this quantity through

$$W^{2}(L) \approx \int_{\frac{3\pi}{L}}^{\pi} dk S(k)$$
 (5.10)

from which the exponent  $\alpha$  may be extracted. Fig.(5.5) shows that  $\alpha$  also saturates for large pinning strengths. Table (5.1) summarises all the above results in a nutshell. The interesting feature one can immediately see is that the hyper-scaling relation



Figure 5.2: Log-Log plot of the width W vs the time for various values of the pinning strength.



Figure 5.3: Plot showing  $\beta$  against the reciprocal of the pinning strength. Notice that  $\beta$  saturates for very large values of pinning.



Figure 5.4: Typical interface profiles with and without the effects of pinning for  $\frac{\Delta}{H} = \frac{1}{3}$  case



Figure 5.5: Plot showing a against the reciprocal of the pinning strength.

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M <sub>maz</sub>	$\beta(M_{max})$	$\alpha(M_{max})$	z(Mmaz)	$\alpha + z$
10	0.100	0.35	3.5	3.85
20	0.121	0.425	3.512	3.937
30	0.146	0.485	3.321	3.806
40	0.156	0.541	3.467	4.00
50	0.162	0.563	3.470	4.03

 $\alpha + \frac{\alpha}{\beta} = 4$  seems to be satisfied to within errors for all the  $M_{max}$  values, although the exponents have different values now. Simulations were also carried out using  $\frac{\Delta}{H} = \frac{1}{2}$ ,

Table 5.1: Growth exponents  $\beta$ ,  $\alpha$  as a function of the maximum pinning strength corresponding to a ratio  $\frac{\Delta}{H} = \frac{1}{3}$ .

which corresponds to a smooth phase with a very small roughening exponent in the absence of pinning (Racz et al., 1991). As before we find that both  $\beta$  and  $\alpha$  saturate for very large pinning values (see Figs. (5.7),(5.8) and (5.9)). Table (5.2) sums up these results, notice that there is no sum relation satisfied in this case. We also see that the value of z jumps from a value of  $\approx 2$ , to much larger values. The  $z \approx 2$  regime as we all know corresponds to a regime where the laplacian  $(\nabla^2 h)$  dominates. It is not very clear at this point as to what controls the relaxation dynamics once the pinning is turned on. There is definitely no  $\nabla^2 h$  term, because this term would certainly dominate all the other terms in the long wavelength limit leading to a  $z \approx 2$ . The fact that the z is very different from 2 indicates a different dynamics. Figs.(5.4) and (5.6) show typical interface configurations with and without pinning for both  $\Delta = \frac{1}{3}$  case, we clearly see that the interface is roughened to a greater extent in the presence of impurities when compared to the pure case, notice the larger hills and valleys in the case of the pinned



Figure 5.6: Typical interface profiles with and without the effects of pinning for  $\frac{\Delta}{H} = \frac{1}{2}$  case



Figure 5.7: Log-Log plot of the width W vs the time for various values of the pinning strength.



Figure 5.8: Plot showing  $\beta$  against the reciprocal of the pinning strength.



Figure 5.9: Plot showing  $\alpha$  against the reciprocal of the pinning strength.

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Mmaz	$\alpha(M_{max})$	$\beta(M_{max})$	$z(M_{max})$
0	0.12	0.054	2.22
10	0.345	0.102	3.41
20	0.44	0.121	3.63
30	0.553	0.128	4.32
40	0.605	0.130	4.65
50	0.626	0.131	4.77

Table 5.2: Growth exponents  $\beta$ ,  $\alpha$  as a function of the maximum pinning strength corresponding to a ratio  $\frac{\Delta}{H} = \frac{1}{2}$ .

pinned case. These correspond to the fact that certain sections of the interface get pinned due to the presence of the background impurity and certain sections don't. The interface tries to adfapt to the random surrounding causing it to make large excursions thus increasing the roughness. The above study should throw light on the roughening dynamics of a driven reconstructing surface in the presence of a quenched impurity and may be the MBE growth process in the presence of impurities.

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# Chapter 6

# Conclusion

# 6.1 Summary

In this thesis we have reviewed various physical properties of interfaces in both equilibrium and nonequilibrium conditions with emphasis on the latter. The kinetic roughening phenomenon of driven interfaces has been studied through several theoretical models. Techniques such as the Renormalization group, Monte Carlo simulation, and direct numerical integration were reviewed and used. Different physical systems may have different surface relaxation mechanisms such as the surface diffusion or desorption which can lead to drastically different surface morphologies at large times. The physical origin of these effects were reviewed and we have focussed our attention on models with surface diffusion as the dominant effect, this is believed to control the growth properties of thin films grown by Molecular Beam Epitaxy.

We have proposed and studied a non-linear model for driven interface dynamics far from equilibrium which is relevant to MBE growth and the roughening of a growing dendrite. The surface evolves into a self-affine structure with scale invariant correlations. We have evaluated the scaling exponents and functions numerically in both d = 1 + 1 and d = 2 + 1 dimensions. For MBE growth, it has been found experimentally that the surface roughness is usually small implying a rather small roughening exponent  $\alpha$ . However, all the previous theoretical models for this process produced

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rather large  $\alpha$ , so large that in some cases the solid-on-solid condition is violated. We have tried to look into this problem by using different nonlinearities in hydrodynamic equations. While the value of  $\alpha$  is indeed reduced somewhat from those of the linear theory, it is still too high to quantitatively account for the experimental findings. Since most nonlinearities are irrelevant for the scaling behavior in the hydrodynamic limit, and the only relevant ones being those that were studied here and in Ref. (Wolf and Villain, 1990; Lai and Sarma, 1991), we may conclude that a nonlinearity would not able to account for the small values of  $\alpha$  and new avenues have to be explored to solve this puzzle. In this regard we note that the only way out would be to modify the noise term in the hydrodynamic equations. All the theoretical models studied so far use additive noise. Experience with stochastic processes however tells us that external noise is usually multiplicative rather than additive. This therefore may provide an explanation and lead to smaller values of  $\alpha$ . It was also found that (Sun, Guo and Grant, 1989) a conserved noise produces a small  $\alpha$ . Thus in the MBE process, one may speculate that the beam flucutations are very small and that the noise is largely internal in origin and hence may be conserved. This scenario however can only be verified experimentally and remains an interesting possibility.

We have also discussed effects of quenched random impurities on the rough aning dynamics of a system with a conservation law. There have been many investigations in this regard but these can only be applied to fluid systems where the fluid interface advances through a random background. Our study is relevant to solid surfaces which are driven out of equilibrium and have impurities trapped near the surface. The conservation law fixes the average interface position, the interface thus experiences the same set of impurities. The breaking of detailed balance ensures that our model is out of equilibrium. We have modeled the random background by putting random pinning strengths at each lattice site. The interface tries to adapt its shape to this random background resulting in a rougher structure. Anomalous roughening exponents were found depending on the pinning strength of the random quenched background. In some cases, the exponents satisfy the same scaling relations as that without the

## CONCLUSION

quenched impurities; and in some others they don't. In all situations, the quenched impurity changes the dynamic universality class the model belongs to. Finally, we note that if the MBE growth is indeed describable by a conserved noise as mentioned above, then this study will provide direct information on what happens if impurities are present in the growth process.

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