Statistics and Dynamics
of Systems Far From Thermal Equilibrium.

Research Proposal for the Ph.D Thesis

Erel Levine

under the supervision of Prof. D. Mukamel

Dept. of Physics of Complex Systems.

Submitted to the Feinberg Graduate School,

Weizmann Institute of Science, Rehovot

January 25, 2001
1 Introduction

Collective phenomena in systems far from thermal equilibrium have been a subject of extensive studies in recent years. Usually these systems are driven out of equilibrium by external fields, such as electric field in the case of conductors, pressure gradient in the case of fluids, temperature gradient in the case of heat conductors, chemical potential gradient in the case of growth problems and many others [1–4]. In many cases these systems reach a steady state, which unlike the equilibrium case, is characterized by non-vanishing currents.

The studies of phase transitions, spontaneous symmetry breaking, and breaking of ergodicity in systems in thermal equilibrium has yielded considerable theoretical understanding over the last five decades. In equilibrium statistical mechanics, one usually associates an energy function, or a Hamiltonian, $\mathcal{H}(C)$ to every possible configuration $C$ of a system. At equilibrium, each configuration $C$ has a weight proportional the Gibbs measure $\exp[-\mathcal{H}(C)/T]$,

$$P_{\text{eq}}(C) = \frac{1}{Z} e^{-\mathcal{H}(C)/T},$$

where $T$ is the temperature and $Z$ the partition function. The problem is then reduced to calculating equilibrium properties by averaging over all configurations weighted by (1).

Under this framework many properties of equilibrium systems, when properly interpreted, are universal. At high temperature, when entropy dominates, matter is isotropic and homogeneous. As temperature is lowered phase transitions to more correlated phases may occur. These transitions may be classified as first order (discontinues), and second order (continuous) transitions. At discontinues transitions, there is the phenomenon of nucleation. Continuous transitions are characterized by the divergence of characteristic lengths, susceptibilities, and relaxation times. At sufficiently low temperatures the system will generally have a lower symmetry than the high temperature phase.

In the study of second order phase transitions the introduction of the renormalization group has provided a method of calculating critical exponents and established that they should depend on the spatial dimension, the symmetry of the order parameter, and the symmetry of the interactions, but not on the detailed form and magnitude of the interaction. Thus, there are universality classes: all transitions in the same universality class have the same exponents.

As the spatial dimension is increased fluctuation become less and less important. Above
a critical dimension, called the upper critical dimension, fluctuations become so unimportant that mean field solutions become valid. However, once the dimension is lower or equal to a critical dimension, called the lower critical dimension, fluctuation can become so violent that they can destroy the ordered state at any finite temperature. Simple arguments have shown that in systems with short range interactions the lower critical dimension is $d = 1$, when the broken symmetry is discrete. When the broken symmetry is continuous the lower critical dimension is known to be $d = 2$.

The dynamics of a system from an initial state towards equilibrium is often described by a master equation of the form

$$ \frac{dP(C)}{dt} = \sum_{C'} M(C, C') P(C') ,$$

(2)

where for $C' \neq C$ the matrix element $M(C, C')dt$ is the probability of a transition from configuration $C'$ to configuration $C$ during the infinitesimal time interval $dt$, and $M(C, C) = -\sum M(C', C)$. To insure that a distribution $P(C)$ evolving according to (2) has a long time limit $P_{st}$ independent of the initial condition, the rule of evolution $M(C, C')$ should be ergodic, i.e. there should be a path of non-zero matrix elements connecting any pair of configurations. Moreover, the simplest way to get $P_{st} = P_{eq}$ is to choose a matrix $M(C, C')$ which satisfies detailed balance, meaning that for any pair of configurations $C_1, C_2$

$$ M(C_1, C_2)P_{eq}(C_2) = M(C_2, C_1)P_{eq}(C_1) .$$

(3)

In contrast, for a nonequilibrium system there is usually no energy function, and the system is defined by its dynamical rules. When the dynamic is ergodic the system usually gets into a steady state, when stationarity, rather then detailed balance, is obtained:

$$ \sum_{C'} M(C', C)P_{st}(C) = \sum_{C'} M(C, C')P_{st}(C').$$

(4)

More generally, nonequilibrium systems can be defined as those evolving through a local stochastic dynamics which does not obey detailed balance with respect to any ‘reasonable’ energy function. By ‘reasonable’ it is meant that the energy function is written down according to microscopic physical principles, and is thus expected to be extensive, to involve local interactions, etc. The main point is that the nonequilibrium system is defined by its dynamics without regard to any concept of energy and it is the dynamics which should seem reasonable or ‘physical’.
Unlike the equilibrium case, a general theoretical framework for studying nonequilibrium phenomena does not exist. One therefore cannot derive similar rules which would be as general as those for equilibrium systems. Rather, one has to resort to studying specific models and probe the resulting types of phase diagrams and phase transitions, with the hope that some general picture might emerge.

A natural way to construct a nonequilibrium steady state is to drive the system by forcing a current of some conserved quantity, for example energy or mass, through the system. Such systems are known as driven diffusive systems (DDS). The archetypical model has been introduced by Katz, Lebowitz and Spohn [5]. Basically it comprises a two dimensional Ising-like lattice gas evolving under conservative Kawasaki dynamics (spin exchange) and with a drive direction imposed. It has been shown that a continuous phase transition exists in the driven system, as is also the case in the undriven (Ising) system, but, most interestingly, one sees generic long range (power-law decay) correlations as opposed to the undriven systems where long-range correlations are only seen at criticality. In this model, as well as in many other driven systems, it is interesting not only to characterize the steady state, but also to investigate the dynamics towards it. We return to this model in more details in Section 2.2.

More recently it has been realized that DDS in one dimension exhibit non-trivial behavior. One of the most striking difference between equilibrium and non-equilibrium systems is the ability of some non-equilibrium systems to sustain long range order, and exhibit spontaneous symmetry breaking (SSB), in one dimension even in the presence of noise. In the last decade several one-dimensional models which show phase transitions as well as SSB have been introduced [6,7]. Similar models are the motivation for Section 3.1 and Section 3.2.

Other nonequilibrium models include reaction-diffusion systems [8,9], surface growth models [4], Directed Percolation (DP) [10] and more. In all these models the concept of universality, borrowed from equilibrium statistical mechanics, has proven to be useful. In particular, the universality class of DP is believed to incorporate vast range of processes which exhibit absorbing-state transitions, as diverse as epidemics, forest fires and transport in random media [10]. In Section 2.1 the existence of universality classes in surface growth models is used to study coarsening processes of striped structures.

The dynamics of cellular processes have attracted much attention in the last decade.
Although vast amount of knowledge has been accumulated by various experimental techniques, the understanding of the mechanisms which govern these processes is scarce. Many of the theoretical studies disregard the fact that cellular processes occur in an environment which is far from thermal equilibrium. Given the breakthroughs of the last few years in experimental techniques, it is proposed that studying cellular processes within the context of nonequilibrium physics may provide some understanding of these processes, as well as some insight about the way nonequilibrium characteristics may be used.

The main purpose of this Ph.D will be to study far from equilibrium systems so that a broad perspective on collective phenomena far from equilibrium systems can be obtained. In particular, special effort would be dedicated to applying methods of statistical mechanics to cellular processes.

In the next section two coarsening scenarios which were studied during the last year are discussed. In the section following that several directions of research which I plan to pursue will be described. A detailed summary of work done so far is given in the appendices in a form of submitted papers.

2 Work Carried Out So Far

Coarsening processes have been extensively studied both experimentally and theoretically over the past decades [11,12]. Most of these studies deal with the way a system approaches its thermal equilibrium state. For a system which can be characterized by a single length scale, say the average domain size $\ell$, it has been shown that under conserving dynamics $\ell \sim t^{1/3}$ while under nonconserving dynamics $\ell \sim t^{1/2}$ [12,13]. These results are independent of the specific details of the system and are thus universal. More recently attention has focused on systems far from thermal equilibrium, driven by an external field [1]. The coarsening processes in these systems towards its nonequilibrium steady state may be rather different from those of systems evolving toward their equilibrium state. For example a study of the evolution of a driven Ising model with conserving dynamics has shown that in one dimension the average domain size grows as $t^{1/2}$ [14] rather than the usual $t^{1/3}$ expected for non-driven systems with conserved dynamics. The presence of the drive introduces a preferred direction in space making the systems inherently anisotropic. In many of these systems this results in striped structures. Typical examples are the stepped structures which occur in surface
growth [15] and wind ripples formed in sand [16]. I present here recent work concerning with the coarsening dynamics of two systems far from thermal equilibrium. The corresponding papers, the first already published and the second submitted, can be found in the appendix.

2.1 Coarsening of a class of driven striped structures


Recently a class of driven models, where phase separation takes place even in one dimension, has been introduced [17–22]. It has been shown that in higher dimensions stripes of alternating types of particles are formed perpendicular to the driving field. The width of the stripes along the direction of the driving field is found to grow as log(t) [23]. This is related to the fact that the interfaces which separate adjacent stripes are macroscopically smooth.

A natural question is as to how the coarsening of stripes is altered when one considers more general scenarios such as, say, non-conserving dynamics or dynamics which leads to rough interfaces separating the stripes. To address these questions we have studied the evolution of driven striped structures. The microscopic dynamics is non-conserving and rough interfaces between the stripes arise.

Without giving the full details of the model, here are its salient features. A microscopic state of the system is given by the configurations of the single valued interfaces separating adjacent stripes. Each interface evolves under local driven dynamics. For example one can consider growth dynamics belonging to the KPZ universality class. All interfaces evolve under the same dynamical rules, and thus, in particular, they all move in the same direction and with the same average velocity. When two interfaces meet at a point, they locally merge to form a single interface. The evolution is such that after some time the entire two interfaces coalesce. This dynamical process is a generalization of the reaction diffusion process $A + A \rightarrow A$, in which diffusing $A$ particles (either with or without a drive) undergo a merging reaction as they collide. In the present generalization the coalescing objects are not particles but extended objects, i.e. the interfaces between stripes.

In studying the model we find that the coarsening process may be well understood by
considering the scaling properties of an isolated interface. We find that the evolution is
different at early and late times. In both regimes the average domain size $\ell(t)$ grows alge-
braically in time. The different regimes, however, are characterized by different exponents.
It is found that at early times the evolution of the width of a single interface dominates the
coarsening process. In this regime the characteristic length scale $\ell(t)$ grows as

$$\ell \sim t^\beta \quad t \ll L^z. \tag{5}$$

Here $z$ and $\beta$ are universal exponents which describe the evolution of the interface width,

$$W = t^\beta f\left(\frac{t}{L^z}\right), \tag{6}$$

where $f$ is a scaling function. At late times the coarsening process is dominated by the
fluctuations in the average position of the interfaces,

$$\ell \sim \frac{t^{1/2}}{L^\varphi} \quad t \gg L^z, \tag{7}$$

where $\varphi = z(1/2 - \beta)$. The values of $\beta$ and $z$ are determined according to the universality
class to which the interfaces belong. In our model the interfaces belong to the KPZ uni-
versality class, except to a single choice of parameters where detailed balance is retained
and the interfaces belong to the EW universality class. We have verified our results in both
cases numerically for one- and two-dimensional interfaces.

### 2.2 Ordering dynamics of the driven lattice gas model

E. Levine, Y. Kafri, and D. Mukamel, Ordering dynamics of the driven lattice gas model , Sub-
mitted to *Phys. Rev. E*; cond-mat/0101324

A bulk of work on driven diffusive systems has focused on a driven Ising lattice gas
model often referred to as the “standard model”, which was introduced by Katz, Lebowitz,
and Spohn [5, 24]. Each of the $L_x \times L_y$ lattice sites is either occupied by a particle or
vacant. Usually the model is studied with equal numbers of occupied and vacant sites.
An external drive is introduced through a field $E$ which biases the motion of the particles
in favor of the $-y$ direction. Imposing periodic boundary conditions causes the field to
generate a current of particles through the system along its direction. The model has been
studied extensively for nearly two decades [1]. The majority of these studies were based
on extensive Monte-Carlo simulations. The phase diagram that emerged consists of two phases: A high temperature phase in which the particle density is homogeneous; and a low temperature phase in which the system orders and phase segregates. Recently it has been conjectured that the Monte-Carlo simulations may be misleading, and in fact the ordered phase for a square system ($L_x \approx L_y$) in the thermodynamic limit may consist of more than a single stripe [25].

Our work has focused on the coarsening of the system from a disordered initial state. We find that for a finite system, the evolution towards a single stripe configuration proceeds through two steps: the formation of stripes, and their coarsening. We argue that the number of stripes at the end of the first step depends on the system aspect ratio and size. Also we show that the coarsening of the stripes becomes slower as the systems size in the direction of the drive is increased. This implies that in the thermodynamic limit a multiple striped configuration is in fact stable.

Using previous results concerning the early-time coarsening of this model [26,27] we have managed to determine that the number of striped initially formed in the system, $m$, is given by

$$m \sim \frac{L_x}{L_y^\phi},$$

(8)

where $\phi \simeq 0.2$. This result implies that for a square system, where $L_x \approx L_y \equiv L$, the number of stripes grows with the system size as $L^{0.8}$. Monte-Carlo simulations verify these results.

To study the latter stage we consider the evolution of the model from a multi-stripe configuration into a single stripe. Using simple scaling arguments we find that the average width of a stripe $\ell$ grows as

$$\ell \sim (t/L_y)^{1/3}.$$

(9)

This implies that a multi-striped configuration is stable in the thermodynamic limit, which is a direct consequence of the fact that the stripes span the entire system and are aligned parallel to the drive. This contrasts the usual coarsening scenario, where the typical size of the domain is independent of the system size. The results are also supported by Monte-Carlo simulations.
3 Plans for Future Studies

In the following I discuss several directions of research which I plan to pursue. A direct continuation of the coarsening models discussed in the previous section is presently under scrutiny. This subject would not be addressed here any further. Rather, I point out some other examples for non-equilibrium issues and collective phenomena which would be addressed.

3.1 Canonical and Grand-Canonical ensembles in non equilibrium statistical mechanics

The notion of different ensembles is well established in equilibrium statistical mechanics. The study of a certain system may become easier by letting some observables to fluctuate, keeping only of its mean values fixed. Under some general constraints, the thermodynamic results remain unchanged when moving from one statistical ensemble to another.

When moving to nonequilibrium systems, the definitions of the different ensembles become vague. Here the dynamics may be inherently non-conserving in terms of either energy or particles. The flow of energy through the systems, and the lack of a definite temperature, may disable fixing even the mean energy or number of particles. In particular, in some systems there is no apparent physical procedure to determine the relative rate between otherwise identical systems of different number of holes.

As in other cases, an insightful lesson can be found in the study of one dimensional systems. Here a framework similar in spirit to the grand canonical ensemble has been proposed [21,28,29]. Indeed, it has been shown that in the thermodynamic limit the fluctuations in the number of particles become negligible. However, clear discrepancy in results of the two ensembles has been found in a certain one-dimensional system [21,22,30]. Also, a comparison of the two ensembles through a model of competing dynamics shows considerable differences [31].

We propose to tackle this issue by considering a simple one-dimensional model with stochastic dynamics, which may be solved exactly both in the canonical and the grand-canonical ensembles. Solving the model in both frameworks would allow the comparison between physical observables, and the way differences between the ensembles come about.
The model is defined on a one-dimensional lattice with a ring topology. In this model, two species of particles, denoted by + and −, occupy half the lattice sites, where all other sites are vacant. The dynamics is defined through the rates
\begin{align}
+0 & \xrightarrow{1} 0+ \\
0- & \xrightarrow{1} -0 \\
+- & \xrightarrow{q} -- ,
\end{align}

where 0 denotes a vacant site. This model is similar to the one studied in [32], but with different boundary conditions. The stationary state of this model is composed of particle clusters with non-trivial distribution of sizes, which changes when \( q \) crosses its mean-field value \( q = 2 \) [29].

### 3.2 Long-range order in quasi one-dimensional model

A similar model to the one introduced in the former section has been studied on a quasi one-dimensional lattice [33]. The model is defined on a periodic \( 2 \times L \) lattice, which may be viewed as two coupled one-dimensional rings. The dynamics within each ring, along \( y \)-bonds, follows (10). In addition, particles hop along \( x \)-bonds into empty sites with rate \( \gamma \).

It has been claimed that in the steady state the quasi one-dimensional model, in contrast to the simple one-dimensional, phase-separates into a single particle cluster of macroscopic size. This claim was supported by numerical simulations [33] and mean-field type analysis [34,35].

The difference in this model between the one-dimensional and the quasi one-dimensional versions is therefore striking. Further investigations as for the roots of this difference are called for. In particular one may ask whether this phase separation exists in the thermodynamic limit, where \( L \to \infty \). Preliminary numerical results indicate that a particle cluster is meta-stable, but not stable, in this limit. We plan to pursue this study, and to investigate the coarsening dynamics in this model.

### 3.3 Wetting transition and Exchange-Bias phenomena

The interaction of a bulk phase of a system with a wall or a substrate may result in wetting phenomena. A layer of a second phase may be formed in the vicinity of the wall, and its thickness may diverge as external parameters, such as temperature or chemical potentials, are varied. Wetting transitions in equilibrium systems has been studied extensively both
theoretically and experimentally [36]. Most of the studies of its non-equilibrium counterparts has focused characterization of the growing phase [37]. recently it has been shown that the wetting transition can be either first- or second-order, and that a coexistence regime between the pinned and growing phase can be found [38,39].

We would like to use these results to study exchange-bias-like phenomena observed in GdFe/TbFe/GbFe domain wall junctions [40]. In such samples previously saturated along the +z direction, the nucleation of reversed magnetization starts from the outer part of a one of the GdFe layers, forming a domain wall (DW). The DW is at first blocked by the TbFe layer, compressed against it, and then propagates into the second GdFe layer.

We propose to study such systems in the framework of non-equilibrium wetting phenomena. In this language one can imagine two phases: a ‘pinned’ phase, where the time for the DW to penetrate the TbFe layer diverges with the system size, and a ‘wet’ phase where the DW propagates thorough the sample. It is also expected that a coexistence regime may be found.

3.4 Statistics and dynamics in cellular processes

In this last section the subject of nonequilibrium phenomena in biological systems is discussed. In many cases, such phenomena have been tackled experimentally, but have not been treated theoretically. It would be interesting to include a system exhibiting non-trivial out of equilibrium behavior in my future studies.

Thermodynamics severs as a key ingredient in understanding molecular biology. For example, thermal motion is considered responsible for bringing molecules together inside the cell, and equilibrium considerations are used to understand processes such as molecular recognition. However, the living cell is a chemical system that is far from equilibrium [41]. By means of a reaction pathway that is determined by enzymes, many reactions are driven in one direction by being coupled to the energetically favorable hydrolysis of ATP to ADP and inorganic Phosphate. The ATP pool is itself maintained at a level far from equilibrium, with a high ratio of ATP over its hydrolysis products. This ATP pool thereby serves as a battery that keeps energy and atoms flow through the cell directed along pathways determined by the enzymes present. For a living system, approaching equilibrium means decay and
death [41].

An interesting question to explore would be in what ways can the cell exploit its nonequilibrium state. For example, Hopfield [42] has shown three decades ago that the specificity with which the genetic code is read in protein synthesis can be increased above the level available from free energy differences in intermediates, if the reaction is strongly but not specifically driven. Protein synthesis, amino-acid recognition, and DNA replication all exhibit the features of Hopfield’s model, termed “kinetic proofreading”. In another, more recent work [43, 44] it has been shown that sensitivity of a biochemical network to variations in biochemical parameters can be reduced to a negligible level in a way which violates severely detailed balance. This has been demonstrated in the context of bacterial chemotaxis.

Recent advances in large scale monitoring of gene expression provide the technology to probe expression kinetics in high resolution [45, 46]. This gives rise to an opportunity to investigate dynamics in the cell theoretically, keeping a close touch with experimental observations. Our first step in this direction is to develop a way to decipher network design from its temporal dynamics. We have suggested and tested both analytically and numerically a method which considers the system response to an external stimulus in order to decipher its network connectivity. This work is in its very early stages. The next step would be to understand the dynamics and statistics of various networks in order to try and figure out basic principles in cellular system design.

**Time periodic phase separation.** An example to a nonequilibrium scenario can be found in cell division mechanism in the bacterium *Escherichia Coli* [47]. Recently it has been shown that the selection of the correct division site relies on a pole-to-pole oscillations of two proteins, MinC and MinD [48, 49]. This oscillating current of the MinCD protein complex survives even through the cell division process, and can be considered as the cell’s steady state.

It is only natural to ask how this scenario comes about. The localization of the MinCD complex at a certain pole can be considered as phase separation. The whole process is therefore time-periodic phase separation in a nonequilibrium system. An interesting task would be to study a model which presents such a behavior, hoping to find predictions which can be verified experimentally.
References


Appendix A

Coarsening of a class of driven striped structures
M.R. Evans, Y. Kafri, E. Levine and D. Mukamel

Appendix B

Ordering dynamics of the driven lattice gas model

E. Levine, Y. Kafri, and D. Mukamel

Submitted to *Phys. Rev. E*; cond-mat/0101324