

Phase Transitions in Nonequilibrium Steady States and Power Laws and Scaling Functions of Surface Growth Processes

Term-paper for PHY563

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Abstract: Three models of surface growth processes in nonequilibrium steady state (NESS): Edwards–Wilkinson Model, Mullins–Herring Model and Kardar–Parisi–Zhang Model, are presented. Power laws, universality of non-equilibrium distributions, and scaling functions are discussed in details together with some experiment results.

I. Introduction

Non-equilibrium systems are many-particle systems which are not in thermal equilibrium. A number of physical systems, usually open systems driven by a strong external force [1], can fall into this class of behavior, for example exciton dynamics [2], and models for self-organized criticality.

Non-equilibrium phase transitions, happening in nonequilibrium systems, have attracted much research on them, mainly for several reasons. Firstly, much deserves being studied about the complex ordering phenomena happening in nonequilibrium systems as nonequilibrium occurs as a more general condition than equilibrium in nature. Secondly, the lack of understanding of the general aspects of nonequilibrium systems expects us to steal some mechanisms from systems in equilibrium, which have been much studied and understood well. Thus, the investigation of the difference and similarities between them would help us discover and understand the properties of nonequilibrium systems well. In addition, power law correlations which are present in many nonequilibrium systems have been shown to be related to equilibrium or nonequilibrium critical phenomena although general mechanisms can allow for these correlations. All these make the research on nonequilibrium phase transitions interesting and fascinating.

In section II, we present a brief and general picture of NESS. Three surface growth processes and their corresponding power laws, and scaling functions are discussed in details in section III.

II. Non-equilibrium Steady States

Non-equilibrium steady states differ from their equilibrium counterparts in that they can admit the presence of fluxes of physical quantities, say, energy or mass, etc. Usually, the fluxes of systems are imposed by boundary conditions, or external driving fields. A well-known example of nonequilibrium steady state is shown in Figure 1[3] in which the boundary conditions emerge as the origin of the fluxes of energy.

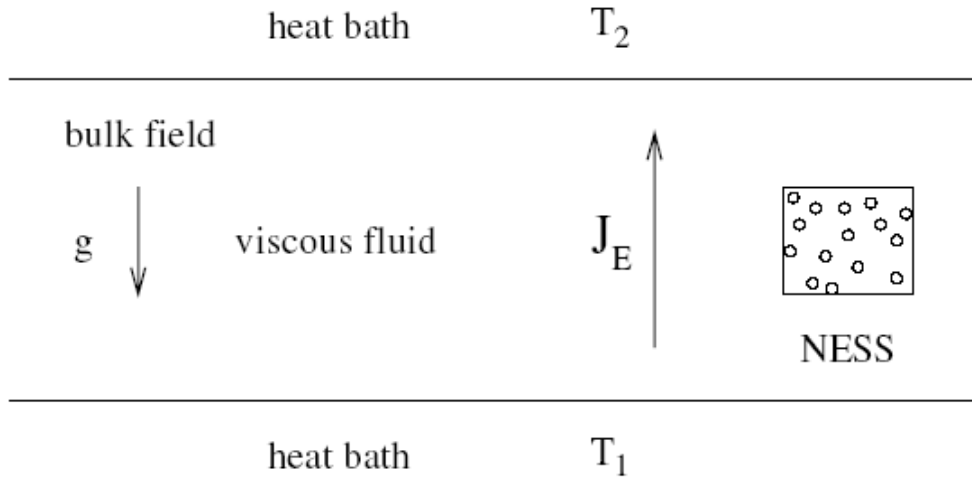


Figure. 1: Setup for Rayleigh-Bénard experiments

It is the famous Rayleigh-Bénard experiment for NESS. The system is composed of two heat baths of temperature of T_1 and T_2 ($T_1 > T_2$) and a horizontal layer of viscous fluid in between. The difference of the two heat bath temperatures works as the driving force of the energy flow. When $T_1 > T_2$, the gradient of the temperature leads to the flux through the system and therefore NESS forms. When $T_1 = T_2$, there is no flux and the system is relaxed to an equilibrium state. The increase of the difference of two bath temperatures would make the system experience a nonequilibrium phase transition, first to a stationary convective pattern, then followed by a series of more complicated patterns.

Let us look at a simple model of spin systems. In equilibrium systems, the dynamics is realized by choosing the next configuration n' from the current configuration n with a probability proportional to the transition rate $W_{n \rightarrow n'}$ that satisfies the detailed balance condition:

$$W_{n \rightarrow n'} P_n = W_{n' \rightarrow n} P_{n'}$$

where n and n' are any two configurations, and $P_n, P_{n'}$ are the probability function that the system takes on configuration n and n' respectively. In

equilibrium systems, P_n is proportional to the Boltzmann weight $f_n = \exp[-\beta E_n]$, where E_n is the energy of configuration n . The detailed balance condition means that there is no mean current of any quantity in the steady state in equilibrium systems. However, in NESS, the presence of the fluxes leads to the breaking of the detailed balance condition, which makes the formation of the theory of the NESS difficult. So, not only the probability function, but also the probability currents in the phase space are needed for the characterization of a NESS.

III. The surface growth processes and power laws and scaling functions

In equilibrium systems, distributions functions are Gaussian and the gaussianity is applicable due to the correlations being short ranged away from critical points. However, the power law correlations lead to non-gaussian distributions. The distribution functions are scaling function at critical points and their shapes are determined by the universality class of critical points.

Similarly, a classification of nonequilibrium distribution functions can be developed. Nonequilibrium universality classes can determine the scaling functions with which we can identify symmetries and underlying mechanisms, just as the same way in the equilibrium systems. Also we can find different systems belonging to the same universality class and common underlying processes present in those systems.

The surface growth processes, as the simplest nonequilibrium systems, fall into universality classes. All processes within one class share the same exponents, and different processes may belong to different universality classes.

In the surface growth, the interface profile is characterized by a height $h(x,t)$, which is a single-valued function and satisfies the Langevin equation:

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

It is the simplest nonlinear equation for a local growth of the surface profile. The first term on the right is the relaxation term of the interface by a surface tension ν , and $\frac{\lambda}{2} (\nabla h)^2$ appears as the lowest-order nonlinear term in the surface growth equation.

High order nonlinear terms can be present, but they won't influence the universal scaling function properties, so we just neglect them in our consideration of scaling properties. The last term $\eta(x,t)$, is the noise which has a Gaussian distribution with $\langle \eta(x,t) \rangle = 0$.

The most important quantities used to characterize the scaling of the interface is the global width parameter $w(L,t)$ defined by

$$w(L,t) = \sqrt{\frac{1}{A_L} \sum_{\vec{r}} [h(\vec{r},t) - \bar{h}]^2}$$

where A_L is the area of the substrate with characteristic linear dimension L , and

$\bar{h} = \frac{1}{A_L} \sum_{\vec{r}} h(\vec{r},t)$ is the average height of the surface. It has been shown [4] that

$w(L,t)$ scales with time t and system size L as: $w(L,t) \sim L^\alpha f(t/L^{\alpha/\beta})$, where

$f(x)$, the scaling function, has the asymptotic form:

$$f(x) \sim \begin{cases} x^\beta, & x \gg 1 \\ const, & x \ll 1 \end{cases}$$

where the exponents α and β are the roughness and the growth exponents respectively.

The steady-state distribution $P(w^2)$ from which any parameter of systems can be derived, is expected to have the scaling form below:

$$P(w^2) \approx \frac{1}{\langle w^2 \rangle} \varphi\left(\frac{w^2}{\langle w^2 \rangle}\right)$$

where $\langle w^2 \rangle$ is the diverging scale, and $\varphi(x)$ is the scaling function characteristic of the universality class for a given surface growth process. Different growth processes may have different scaling function characteristic of NESS. Below, we will discuss several main surface growth processes: Edwards–Wilkinson (EW) and Mullins–Herring (MH), which are linear, and Kardar–Parisi–Zhang (KPZ) which is nonlinear, and their scaling functions.

A. Edwards–Wilkinson Model (EW)

The Edwards-Wilkinson equation [5], based on Langevin type equation, was the first continuum equation used to study the growth of interface by particles deposition. The nonlinear term isn't considered in the equation and it has the following form:

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

From the equation, we have the exact values of the scaling exponents [6]:

$$\alpha = \frac{3-d}{2}, \quad \beta = \frac{3-d}{4}, \quad z = \frac{\alpha}{\beta}.$$

Where d is the dimension of the system, and z represents the dynamical exponent.

The linear EW equation is exactly solvable and the solution in one dimension is:

$$\varphi(x) = \frac{\pi^2}{3} \sum_{n=1}^{\infty} (-1)^{n-1} n^2 \exp\left(-\frac{\pi^2}{6} n^2 x\right)$$

which is shown in Figure 2 [3]. An exponential decay $\varphi(x) \sim e^{-\pi^2 x/6}$ is displayed at large x and for $x \rightarrow 0$, $\varphi(x) \sim x^{-5/2} e^{-3/(2x)}$, showing an essential singularity. With $\varphi(x)$, we can determine the universality class for a given process.

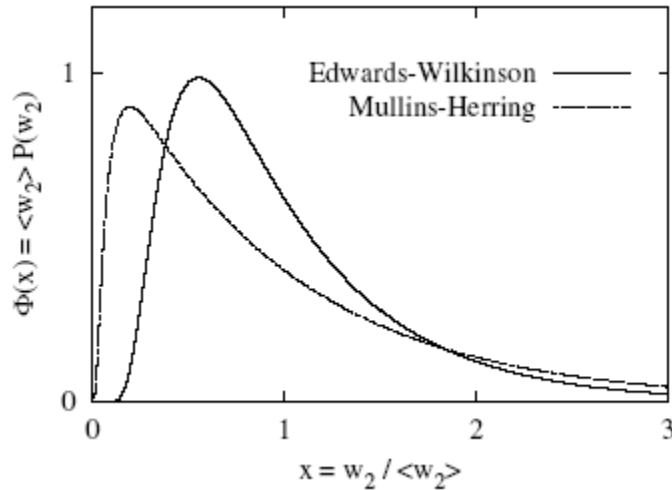


Figure.2: the scaling function of the EW and MH models in one dimension

B. Mullins–Herring Model (MH)

Mullins–Herring Model is also called curvature driven growth process where the

rearrangement of deposited particles is driven by surface diffusion and the particle current is towards places with many neighboring particles. The diffusion current depends on the curvature of the surface: $j \propto \nabla(\nabla^2 h)$, and the equation can be written as

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

according to the conservation law [3]. Just like the EW equation, this equation can be solved exactly, leading to the exponents $\alpha = 1$, $\beta = \frac{1}{4}$ and $z = 4$ in (2+1) dimension [7].

Figure 3 [7] show the dependence of $\varphi(x)$ on the scaled variable $w^2 / \langle w^2 \rangle$ for a thick Ag film with different L in the one-dimension and two-dimension MH models.

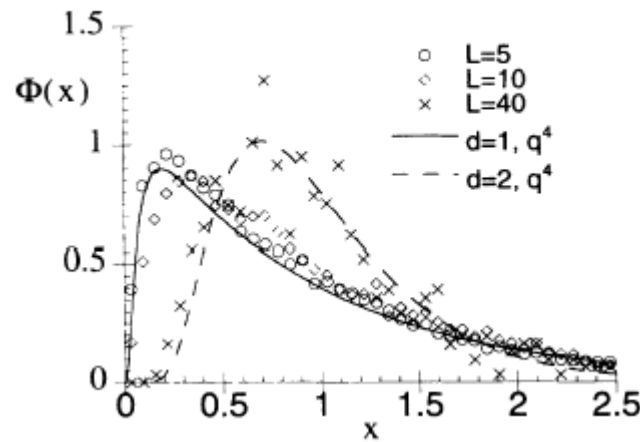


Figure.3: the calculated scaling function for L=5, 10 and 40nm for a 702 nm thick Ag film for one and two dimension models

And, in experiments, AFM and STM measurements of the profile of a film can help determine the distribution function and therefore the corresponding universality class.

The comparison of the EW and MH distribution function curves in one dimension is shown in Figure 2. From the graph, the surface described by the MH equation is distinct from the EW growth as far as the universality classes they belong

to. The differences of their maximum, their decay when x is large, and their small cutoff make them behave differently in the vicinity of critical points.

C. Kardar–Parisi–Zhang Model(KPZ)

The KPZ model is defined through the Langevin equation:

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

This model, together with EW model, is the two of early widely used continuum models of growth and deposition models. Their main difference is that the KPZ model consider the nonlinear term in the above equation while the EW model just ignore it which means in KPZ model growth occurs in a direction locally perpendicular to the existing surface.

The nonlinearity of the KPZ equation makes its exact solution impossible. Numerical solutions [8] give to $\alpha = \frac{1}{2}$ and $z = \frac{3}{2}$ for one dimension(exact solution), and $\alpha \sim \frac{1}{2}$ and $z \sim \frac{3}{2}$ for two dimension, and expect to have $z = 2$ for higher dimension. The KPZ equation contains three different universality classes: the first corresponds to the random deposition model [9] with $h \sim t^{1/2}$ when $\nu = \lambda = 0$, and the second is the ideal interface [5] with $z = 2$ and $\alpha = (2-d)/2$ when $\lambda = 0$, the last one is a new universality class with $\alpha = \frac{1}{2}$ and $z = \frac{2}{3}$ for $\lambda \neq 0$.

Figure 4. [10] shows power spectral density (PSD) (or surface power spectrum) plots of the surface morphology at different times for films grown with Chemical Vapor Deposition, and Figure 5 [10] displays the measured surface width change with time. For $t < 50 \text{ min}$, $\beta_{II} = 0.42 \pm 0.04$; for $50 \text{ min} < t < 15 - 30h$, $\beta_{III} = 0.26 \pm 0.03$, and for $t > 30h$, the width saturates. The experimental results $\alpha_{III} = 0.42 \pm 0.03$, $\beta_{III} = 0.26 \pm 0.03$ and $z = 1.6 \pm 0.1$, are consistent with the approximate exponents in three dimension KPZ model, $\alpha_{KPZ} = 0.39$, $\beta_{KPZ} = 0.24$ and $z_{KPZ} = 1.63$ [4], within experimental errors, and indicates that the CVD growth process is a KPZ class.

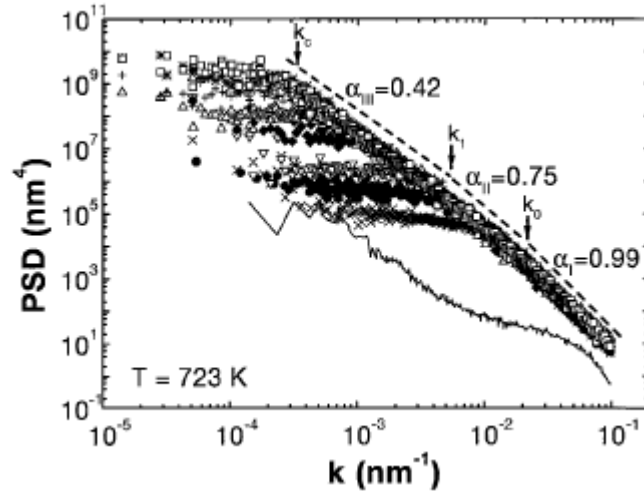


Figure.4: PSD curves from AFM images of the SiO₂ surface at different times

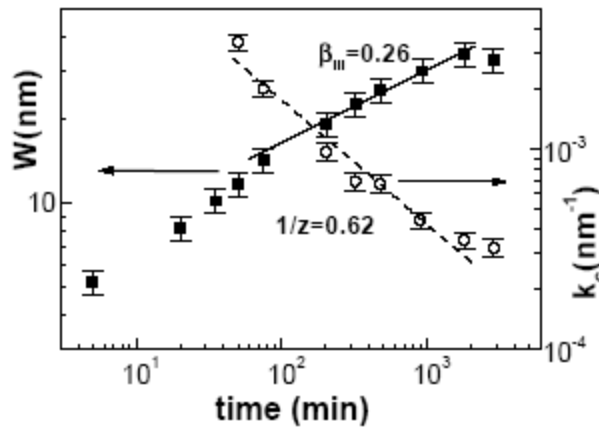


Figure.5: Plot of $w(t)$ with time. The slopes of the solid and dashed lines are,

$$\beta_{III} = 0.26, \text{ and } 1/z = 0.62, \text{ respectively.}$$

Simulation results of the scaling function are displayed in Figure 6 [3]. From the graph, we can see, with the increase of d , the scaling function gets narrower and more centered on $x = 1$, and this tendency continues for high d .

The nonlinear term makes the surface of the KPZ model rough or critical, and results in many interesting phenomena and many issues which still remain unsolved. The question of upper critical dimension is one of controversial topics.

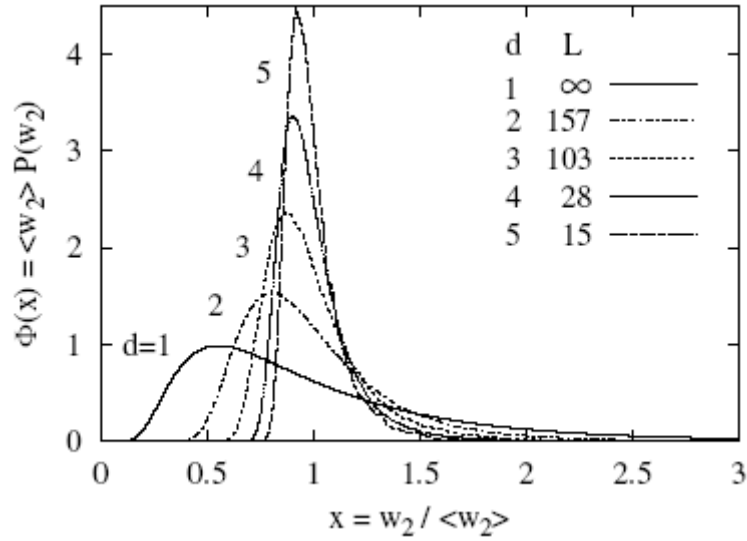


Figure.6: the scaling function for KPZ steady-state surfaces in dimension 1-5

IV. Conclusion

We introduced the general concept of nonequilibrium process and particularly nonequilibrium phase transition using models that describe surface growth phenomena. Power laws, and scaling functions, appearing as useful tools, help us distinguish and understand these models by assigning them different universality classes. Also, experiments show compatible results with theoretical simulation and calculation.

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