Internal Fluctuations Effects on Fisher Waves

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We study the diffusion-limited reaction $A + A \leftrightarrow A$ in various spatial dimensions to observe the effect of internal fluctuations on the interface between stable and unstable phases. We find that, similar to what has been observed in $d = 1$ dimensions, internal fluctuations modify the mean-field behavior predictions for this process, which is given by Fisher’s reaction-diffusion equation. In $d > 1$ the front displays local fluctuations perpendicular to the direction of motion which, with a proper definition of the interface, can be fully described within the Kardar-Parisi-Zhang (KPZ) universality class. This clarifies the apparent discrepancies with KPZ predictions reported recently.

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Fluctuations in the macroscopic behavior of reaction-diffusion (RD) systems could play an important role whether these fluctuations are produced by the discrete nature of the elementary constituents (internal) or by environmental random variations (external). Often both types of fluctuations are neglected in the theoretical treatment, thus describing the system by an action-mass type equation (mean-field approximation). Fluctuations in RD systems can, for instance, give rise to instabilities (1), modify the reaction front velocity (2,3), allow the system to reach new states absent in the mean-field description (4), or produce spatial correlations in the system which in turn can dominate the macroscopic system behavior (5).

While these effects appear in different situations, there is a theoretical and experimental interest in the problem of front propagation in RD systems. The simplest example is that of invasion of an unstable phase by a stable one, which at the mean-field approximation level is described by Fisher’s equation (6):

$$\frac{\partial \rho}{\partial t} = D \nabla^2 \rho + k_1 \rho - k_2 \rho^2$$

where $\rho(x, t)$ is the local concentration ($x \in \mathbb{R}^d$) characterizing the system. Equation (1) arises in the macroscopic description of many processes in physics, chemistry, and biology and is a generic model for reaction front propagation in systems undergoing a transition from a marginally unstable ($\rho = 0$) to a stable ($\rho_{eq} = k_1/k_2$) state. Thus, for initially segregated conditions, i.e. $\rho(x) = \rho_{eq}$ for $x_1 \leq 0$ and $\rho(x) = 0$ for $x_1 > 0$ (with $x = (x_1, x_\perp)$, $x_1 \in \mathbb{R}^d$, $x_\perp \in \mathbb{R}$ and $d = d_1 + 1$), the solution of (1) is a front invading the stable phase and propagating along $x_\perp$ with a constant velocity $v \geq v_{min} = 2(k_1 D)^{1/2}$ which is selected depending on the initial condition according to the “marginal stability criterion” (7).

At the same time, the front broadens until it reaches a finite width $\xi \simeq 8(D/k_1)^{1/2}$.

The question of how faithfully continuum equation (1) resembles the macroscopic front dynamics of microscopic RD discrete systems has drawn a lot of attention recently. In particular, much attention has been devoted to microscopic stochastic models like $A + A \leftrightarrow A$ or $A + B \rightarrow 2A$, where $A$ and $B$ are active species. Discreteness of those systems is responsible for fluctuations in $\rho(x, t)$ and introduces an effective cutoff in the reaction-rates which modifies the properties of the front. Most of the studies have concentrated on observing how the microscopic system approaches the macroscopic behavior described by Eq. (1) in $d = 1$ when $N \to \infty$, where $N$ is the number of particles per site (8). Using van Kampen’s system size expansion (9) or field-theory techniques (10), the macroscopic dynamics of the microscopic Master equation can be expressed in terms of a Langevin equation which, in the case of the $A + A \leftrightarrow A$ scheme, reads (10):

$$\frac{\partial \rho}{\partial t} = D \nabla^2 \rho + k_1 \rho - k_2 \rho^2 + \sqrt{(k_1 \rho - k_2 \rho^2)} \eta(x, t)$$

where $\eta(x, t)$ is a uncorrelated white noise, $\langle \eta(x, t) \rangle = 0$, $\langle \eta(x, t) \eta(x', t') \rangle = 2N^{-1/2} \delta(x - x') \delta(t - t')$, and $N$ is a reference level of number of particles, which is proportional to $N$. In the limit $N \to \infty$, the noise term in (2) (which reflects the fluctuations in the number of particles) vanishes and we recover (1). In this limit, the effective cutoff in the reaction term imposed by the discreteness seems to be the leading contribution, and it is possible to derive corrections to the velocity which yield the well known result $v - v_{min} \sim 1/\log^2 N$ (10).

The purpose of this paper is to extend this analysis of discrete microscopic models to higher dimensions. In $d \geq 2$ the front position is given by an interface at $x_1 = h(x_\perp, t)$ which separates the stable from the unstable domain. Due to the microscopic fluctuations one expects the interface to roughen and its fluctuations to be described asymptotically by the Kardar-Parisi-Zhang (KPZ) (11) equation, which features the simplest and most relevant non-linearity (in the renormalization group sense) that considers local and lateral growth:

$$\frac{\partial h}{\partial t} = \bar{v} + \bar{D} \nabla^2 h + \frac{\lambda}{2} (\nabla \cdot h)^2 + \sqrt{2\sigma} \eta_\perp(x_\perp, t)$$

where $\eta_\perp(x_\perp, t)$ is an uncorrelated white noise, and $\nabla \cdot$ is the divergence operator defined over the substrate $x_\perp$. The interface is described by its mean position $\bar{h}(t)$ and its roughness,
where $\langle \cdots \rangle$ means average over different realizations and the bar denotes average over the substrate $x_1 \in L_{d_\perp}$ ($L_{d_\perp}$ is substrate lateral length). As it is well known, in the KPZ equation $w$ obeys a scaling form $w(L_{d_\perp},t) = t^{d/2} f(t/L_{d_\perp}^d)$, where $w \sim t^d$ if $t \ll L_{d_\perp}^d$ and $w = w_{\text{sat}} \sim L_{d_\perp}^d$ if $t \gg L_{d_\perp}^d$, where $\alpha = \beta z$ is the roughness exponent [12].

However, studies of microscopic realizations of Eq. (1) have questioned the applicability of (3) to describe the processes in Fig. 1a which, in the mean-field approximation, $\mu$ is the largest value of $x_\parallel$ inside the stable domain for fixed $x_1$ [13].

Simulations show that the interface advances linearly in time, $\bar{h} = vt$, where from we can extract the velocity of the front in any dimension. Values obtained are reported in Fig. 1b and compared with the deterministic prediction $v = v_{\text{min}} = 2\sqrt{D\mu}$ of Eq. (1). We recall that in $d = 1$ the stochastic model admits an exact solution [17], and the front advances with velocity $v = D\mu$. The difference between both expressions reflects the importance of fluctuations when $N = 1$ and $d = 1$, and agrees with the breakdown of the approximation $v - v_{\text{min}} \sim \log^2 N$ when $N = 1$. Interestingly, for $d > 1$ we recover the law $v \sim \mu^{1/2}$, although the value is still corrected due to the fluctuations in the number of particles. Nevertheless, the velocity change is smaller when the dimension is increased, as fluctuations get averaged over the transverse dimensions. Moreover, assuming that Eq. (3) holds, we can obtain the value of $\lambda$ by tilting the substrate with an overall slope $m$ and measuring the velocity. As expected we obtain $v(m) = v(0)(1 + m^2, \lambda = v(0)$ [12].

For $d = 2$ the interface roughens subject to internal fluctuations, and the roughness grows like $w(t) \sim t^3$ until it saturates to a constant value $w_{\text{sat}} \sim L_{d_\perp}^\alpha$ (see Fig. 3). When $\mu = 0.1$ we obtain $\beta_{d_\perp} = 0.27 \pm 0.01$ and $\alpha = 0.40 \pm 0.01$, consistent with [13]. Nevertheless, a closer inspection of the data suggests that there is a crossover from non-Gaussian fluctuations at small scales to Gaussian ones at large scales. Although this crossover could be guessed, for instance, from the value of $w_{\text{sat}}(L_{d_\perp})$ for $\mu = 0.1$ (which is seen to change its slope in a log-log plot), it becomes clearer if we look
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here, the noise term scales as $\rho^{1/2} n(x, t)$ for $\rho \to 0$ [see Eqs. (3) and (4)]. Thus, even if the parallel dimension is relevant to determine the interface properties of the front for large values of $N$, we expect internal fluctuations to give a different universality class from the one proposed in [10].

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The specific choice of the microscopic rules, as long as the mean-field limit of them coincides with (1). It has been shown that with a proper definition of the interface, microscopic realizations of Fisher’s equation with $N$ mean-field limit of them coincides with (1).

In summary we have studied two microscopic stochastic realizations of Fisher’s equation with $N = 1$. It has been shown that with a proper definition of the interface, long-wavelength fluctuations are fully described within the KPZ scaling in $d_{\perp} = 2$. $S(q) \sim q^{-2+2\alpha}$ with $\alpha = 0.393$. Inset: Saturation roughness as a function of $L_{\perp}$ in $d = 4$. Dashed line corresponds to the power law $L_{\perp}^\alpha$ with $\alpha = 0.313$.

The absorbing state ($\rho_{eq} = 0$) for $d \leq 4$ [20]. In this case, the mesoscopic dynamics of the system are given by

$$\frac{\partial \rho}{\partial t} = D \nabla^2 \rho + k_1 \rho - k_2 \rho^2 + \sqrt{k_3 \rho} n(x, t),$$

the only difference with (3) being the form of the noise term. Away from the transition point (which occurs when $\mu = 0.22 \pm 0.01$ for fixed value of $c = 0.1$), interface fluctuations behave similarly to the previous model (see Fig. 3b), confirming that our results do not depend on the specific choice of the microscopic rules, as long as the mean-field limit of them coincides with (1).

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Note that $N$ has to be finite, because in the limit $N \to \infty$, noise terms in (3) and (4) vanish and hence the interface does not fluctuate.

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