Macroscopic Response to Microscopic Intrinsic Noise in Three-Dimensional Fisher Fronts

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We study the dynamics of three-dimensional Fisher fronts in the presence of density fluctuations. To this end we simulate the Fisher equation subject to stochastic internal noise, and study how the front moves and roughens as a function of the number of particles in the system, N. Our results suggest that the macroscopic behavior of the system is driven by the microscopic dynamics at its leading edge where number fluctuations are dominated by rare events. Contrary to naive expectations, the strength of front fluctuations decays extremely slowly as $1/\log N$, inducing large-scale fluctuations which we find belong to the one-dimensional Kardar-Parisi-Zhang universality class of kinetically rough interfaces. Hence, we find that there is no weak-noise regime for Fisher fronts, even for realistic numbers of particles in macroscopic systems.

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Microscopic fluctuations can play an important role in the macroscopic behavior of reaction-diffusion (RD) systems. Although usually neglected in theoretical descriptions they can, for instance, give rise to instabilities [1], allow the system to reach new states which are not available in the deterministic description [2,3], or produce spatial correlations which in turn dominate the macroscopic system behavior [4,5]. This is particularly true at onset for transitions from metastable or unstable phases, in which microscopic noise due to thermal or density fluctuations can be amplified to macroscopic time and length scales [6,7]. A prominent context, both from the experimental and from the theoretical points of view, is provided by front propagation in RD systems, as in the invasion of an unstable phase by a stable one [8]. For deterministic systems, this is paradigmatically described by the Fisher-Kolmogorov-Petrovsky-Piscunov (FKPP) equation [9–11],

$$\frac{\partial \rho}{\partial t} = D\Delta\rho + \rho - \rho^2, \tag{1}$$

where $\rho(\boldsymbol{x}, t)$ represents, e.g., the concentration of particles in the system. Here, $\boldsymbol{x} = (x_\perp, \boldsymbol{x}_\parallel) \in \mathbb{R}^d$, $x_\perp \in \mathbb{R}$, $x_\parallel \in \mathbb{R}^{d_\parallel}$, and $d = d_\parallel + 1$. Frequently, the ρ axis provides an additional physical dimension. In such a case, the Euclidean dimension of the full system is $d_E = d + 1 = d_\parallel + 2$. Indeed, Eq. (1) provides the macroscopic description of many processes in physics [12], chemistry [13], and biological evolution [14,15], being a generic model for reaction-front propagation in systems undergoing a transition from a marginally unstable ($\rho = 0$) to a stable ($\rho_{\mathrm{eq}} = 1$) state. Thus, for initially segregated conditions, i.e., $\rho(\boldsymbol{x}) = \rho_{\mathrm{eq}}$ for $x_\perp \leq 0$ and $\rho(\boldsymbol{x}) = 0$ for $x_\perp > 0$, the solution of Eq. (1) is a traveling-wave (front) that invades the unstable phase by propagating along $x_\perp$ with a constant velocity $v \geq v_{\min} = 2D^{1/2}$, which is selected according to a "marginal stability" criterion [16].

The behavior of FKPP fronts can be explained by the dynamics at their edge, i.e., in the region where $\rho \simeq 0$ [2,16]. Here, FKPP waves become extremely sensitive to microscopic perturbations, due to the logistic-growth mechanism in Eq. (1). Specifically, FKPP waves are severely affected by density fluctuations around $\rho \simeq 1/N$, where N is the number of particles in the system; thus, the front velocity changes to $v_N \simeq v_{\min} - v_{\min}(C/\log^2 N)$, where $C > 0$. Even at a macroscopic level, i.e., when N is similar to the Avogrado number, this correction remains significant, exemplifying the strong impact that fluctuations due to particle discreteness can have on the dynamics of traveling waves [15]. This result has been confirmed in particle models described at a mean-field level by the FKPP equation [2,6,7,17], and in the stochastic FKPP (sFKPP) equation,

$$\frac{\partial \rho}{\partial t} = D\Delta\rho + \rho - \rho^2 + \sqrt{\rho(1-\rho)/N}\,\eta(\boldsymbol{x}, t). \tag{2}$$

Equation (2) is the minimal continuum description of some particle RD models [7,12] which includes density (intrinsic) fluctuations, η being a Gaussian white noise of unit variance. Indeed, for, e.g., the $A \rightleftharpoons 2A$ model, the sFKPP equation has been explicitly derived through various approaches [18–22]. While an effective cutoff theory [2] and heuristic arguments on fluctuations at the front tip [23] anticipated the noise-induced contribution to v_N, numerical integration of Eq. (2) in $d = 1$ [24], and, more recently, an exact proof [21], both indeed found the $1/\log^2 N$ correction. The strong noise regime of Eq. (2) attests to even more drastic changes in the form of the velocity [22,25].

Several authors have studied whether this sensitivity of FKPP waves to intrinsic fluctuations does also translate into higher-order perturbations for $d > 1$ fronts. Specifically, FKPP fronts were conjectured in [26] to be so strongly affected by noise that the $d_\parallel$-dimensional front interface would show fluctuations compatible with those of the Kardar-Parisi-Zhang (KPZ) universality class of kinetically rough d-dimensional surfaces [27]. Thus, FKPP fronts would behave like interfaces in a higher dimension, as suggested by preliminary simulations of the $A \rightleftharpoons 2A$ model in $d_\parallel = 1$ [28,29]. However, this effect was later shown to disappear at large scales in those particle models [17], recovering the KPZ universality class in the appropriate dimension. In any case, particle simulations were performed far away from the regime in which Eq. (2) is a good representation for the particle model [17], namely, where the number of particles N is large. Thus, currently a clear understanding on the effect of intrinsic noise on macroscopically large FKPP fronts is still lacking for $d > 1$, especially for the important $d = 2$ and $N \gg 1$ setting of most real-life experiments.

In this Letter we show that fluctuations in the advancing two-dimensional front described by the sFKPP equation in $d = 2$ ($d_E = 3$) are controlled by the leading one-dimensional (1D) "contact line" defined by the $\rho \simeq 1/N$ condition. While inducing 1D KPZ statistics, this implies that it is microscopic density fluctuations which actually control the evolution of the macroscopic front. Specifically, we perform numerical simulations of Eq. (2) for different N and study how the interface fluctuations depend on this parameter. We employ a special algorithm introduced in [24,30,31]. It is based on a splitting step method which numerically integrates stochastic partial differential equations. Specifically, at each time step the stochastic part of Eq. (2) is integrated exactly and the result is fed into a standard deterministic numerical integration of the FKPP equation, Eq. (1). Mathematical analysis in [30] showed that the algorithm preserves non-negativity and that it converges to the solutions of the stochastic Eq. (2). More importantly, the computation time depends only weakly on the order of magnitude of N, unlike in particle models. This algorithm was already used in [24], where it confirmed the Brunet-Derrida velocity correction for the $d = 1$ front dynamics.

We have simulated the sFKPP equation on a grid of size $L_\perp \times L_\parallel$ for different values of $L_{\perp,\parallel}$. As an initial condition we have taken a step function, $\rho(x_\perp, x_\parallel, 0) = \Theta(x_\perp)$. We follow the *front* interface defined by the equipotential line $x_\perp = h_f(x_\parallel, t)$, where $\rho(h_f(x_\parallel, t), x_\parallel, t) = 1/2$. As fluctuations become dominant at values $\rho = 1/N$, we also define the edge interface $h_e(x_\parallel, t)$ by the equipotential line where $\rho(h_e(x_\parallel, t), x_\parallel, t) = 1/N$, see Fig. 1. For very large N (or small noise), the front shape away from the tip is well described by the solutions of Eq. (1). In particular, using the fact that these decay as $\rho \sim e^{-[x_\perp - h_f(x_\perp, t)]/\sqrt{D}}$, we get that the distance between the edge and the front scales as $h_f - h_e \sim \sqrt{D} \log N$ [1].

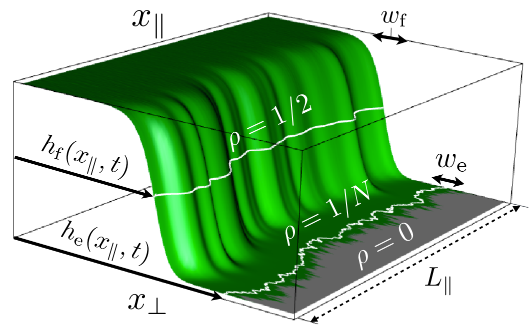

FIG. 1 (color online). FKPP front in $d_E = 3$, as obtained by numerical simulations of Eq. (2), with indication of notation and quantities introduced in the text. White lines correspond to equipotential lines at $\rho = 1/2$ (front interface) and $\rho = 1/N$ (edge interface).

Both $h_f(x_\parallel, t)$ and $h_e(x_\parallel, t)$ are one-dimensional interfaces that travel in time with a constant velocity (which is given by v_N, results not shown), but which also roughen as a result of noise fluctuations. To assess these dynamics [27], we study the roughness of the interface $w^2(t) = \langle [h(x_\parallel, t) - \bar{h}(t)]^2 \rangle$, and the structure factor $S(q) = \langle \hat{h}_q(t) \hat{h}_{-q}(t) \rangle$, where $\hat{h}_q(t)$ is the Fourier transform of $h(x_\parallel, t) - \bar{h}(t)$, the bar denotes space average over $x_\parallel$, and $h = h_{f,e}$. Our simulations show (see Fig. 2) that interface fluctuations are very large, even for small noise.

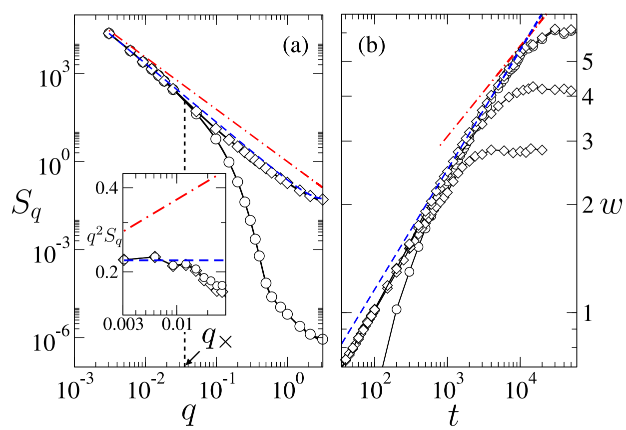

FIG. 2 (color online). (a) Structure factor of the front (circles) and edge (diamonds) interfaces, together with the behavior of the 1D (blue dashed) and 2D (red dot-dashed, asymptotic) KPZ behaviors. System size is $L_\parallel = 1024$. Inset: rescaled structure factor $q^2 S_q$ as a function of q. For small q, the front and edge interfaces both show 1D KPZ behavior $S_q \sim q^{-2}$. Lines correspond to those in the main panel. (b) Time evolution of the roughness of the edge interface for $L_\parallel = 2048, 1024$, and 512 (diamonds, top to bottom) and roughness of the front interface for $L_\parallel = 2048$ (circles) compared to the 1D (blue dashed) and 2D (red dot-dashed) KPZ scaling behavior. In all cases $N = 10^6$. Solid lines are guides to the eye. All units are arbitrary.

In fact, $S(q,t)$ coincides for both interfaces at small $q < q_\times$, which means that, although $h_f(x_\parallel, t)$ is much smoother than $h_e(x_\parallel, t)$ at small spatial scales $q > q_\times$ (see Fig. 1), both interfaces display the same large-scale fluctuations. We find that the characteristic distance above which both interfaces display the same fluctuations scales as $1/q_\times \sim \log N$ (see Fig. 4). This can be intuitively expected, as it coincides with the actual distance separating the two interfaces. Much beyond that characteristic length, the *internal* 2D structure of the front becomes irrelevant, as it is perceived as a one-dimensional object.

Furthermore, these large-scale fluctuations are well described by the KPZ universality class for one-dimensional rough interfaces. In particular, we find that $S(q) \sim 1/q^{2\alpha+1}$ with $\alpha \simeq 1/2$, and $w^2(t) \sim t^{2\beta}$ with $\beta \simeq 1/3$ [27]; see dashed lines in Fig. 2. Indeed, 2D KPZ behavior characterized by $\alpha \simeq 0.39$ and $\beta \simeq 0.24$ [32] provides a much poorer description of the numerical data; see the respective dot-dashed lines in Figs. 2(a) and 2(b). This result corroborates the finding in [17]: fluctuations of $d_\parallel$-dimensional FKPP fronts indeed belong to the KPZ universality class for $d_\parallel$-dimensional interfaces. But it also highlights a potential problem with system size: for large q, fluctuations of $h_f(x_\parallel, t)$ are very small and the asymptotic KPZ regime is only achieved for very large system sizes.

The relationship between $h_f(x_\parallel, t)$ and $h_e(x_\parallel, t)$ does not only happen at large scales for aggregated variables like $w^2(t)$ and $S(q,t)$. Motivated by the phenomenological theory in [23], in which the fluctuations of the $d = 1$ front position in the sFKPP equation were explained by large and rare fluctuations at the front edge, we study how the fluctuations of the front and edge interfaces are related. Figure 3(a) shows the dynamics of the roughness $w(t)$ of both interfaces, for a single noise realization. As we can see, the large-scale fluctuations of $h_f(x_\parallel, t)$ come closely behind those at the edge, which suggests that any disorder that microscopically happens at the edge propagates back and eventually occurs at the front interface. To measure the time delay between these events, we have computed the cross-correlation between the $w(t)$ time series at both interfaces, $\mathrm{CCF}(\tau) = \tilde{w}_f * \tilde{w}_e[\tau] = \sum_t \tilde{w}_f(t)\tilde{w}_e(t+\tau)$, where $\tilde{w}_i(t)$ is the normalized unit-variance and zero-mean time series constructed from $w_i(t)$. The CCF has a peak at a time lag $\tau = \Delta$, which depends on N. An accurate regression yields $\Delta \sim \log^\gamma N$, where $\gamma = 1.97 \pm 0.03$, see Figs. 3(b) and 3(c). Interestingly, this time scale has the same scaling as the relaxation time of perturbations in $d = 1$ FKPP fronts found in [33], which could explain the origin of the former: fluctuations produced at the edge of the front propagate into the macroscopic front $h_f(x_\parallel, t)$ within a time which is set by the relaxation rate of fluctuations in the system. These findings suggest a similar picture to the one found in [23] for one less dimension: the fluctuations of $h_f(x_\parallel, t)$ are dominated by those at $h_e(x_\parallel, t)$,

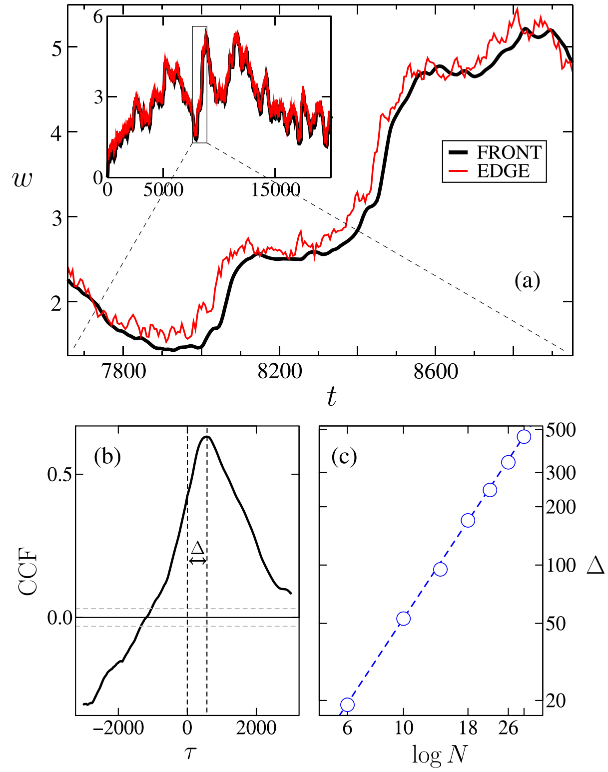

FIG. 3 (color online). (a) Roughness time series for the edge (thin red solid line) and front (thick black solid line) interfaces, for a single noise realization. Inset: Full dynamics. (b) Cross-correlation function between front and edge roughness time series, for a single noise realization and $N = 10^{30}$. The time to the first maximum defines the lag Δ; see main text. (c) Values of Δ (circles) for different values of N, and $L_y = 512$. The line is a fit to $\Delta \sim \log^\gamma N$, where $\gamma = 1.97$. Statistical errors are smaller than the symbol size. All units are arbitrary.

which in our case turn out to be described by the 1D KPZ universality class.

Finally, we study how front fluctuations depend on the strength of the noise, $1/N$. To this end we compare the $S(q)$ curves obtained for different values of N. We find (see Fig. 4) that data can be collapsed in the small-q region using N-dependent factors A_N and B_N, such that $S(q)/A_N = f(qB_N)$, where $f(x)$ is an N-independent function that behaves as $f(x) \simeq C/x^2$ for small arguments. Moreover, from Fig. 4(b) we find $A_N, B_N \sim \log N$, which justifies in particular that $q_\times$ as defined in Fig. 2 scales as $q_\times \sim 1/\log N$. Furthermore, $S(q) \sim CA_N/(B_N^2 q^2)$, suggesting that the interface feels an effective "temperature" (fluctuations strength) $T_{\mathrm{eff}} = CA_N/B_N^2$ and, hence,

$$T_{\mathrm{eff}} \sim \frac{1}{\log N}. \tag{3}$$

The effective temperature of FKPP fronts thus decays very slowly as $N \to \infty$. Note that, even at Avogrado numbers of particles $N \simeq 10^{23}$ for which microscopic noise might be

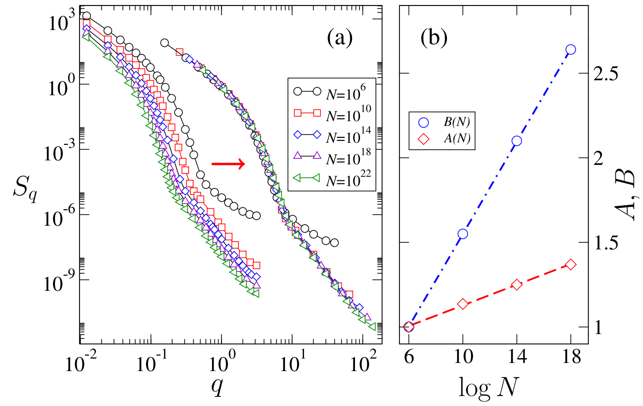

FIG. 4 (color online). (a) Structure factor of the front interface for different values of N, together with rescaled curves obtained by collapsing all curves to the $N = 10^6$ data in the macroscopic region $q \ll 1$; see main text for details. (b) Rescaling factors of S_q and q as functions of N (symbols) together with linear fits (lines). Statistical errors are smaller than the symbol size. All units are arbitrary.

expected to be negligible, we get a value for $T_{\rm eff}$ that is still moderate and implies observable macroscopic fluctuations. Once again, fluctuations in FKPP equations produce strong corrections to the expected deterministic behavior.

In summary, we have studied the macroscopic fluctuations of Fisher fronts in the relevant, real-life context of three Euclidean dimensions. What we have found is that the modification to the front velocity due to microscopic fluctuations, as anticipated by Brunet and Derrida [2], is not the only strong correction to the dynamics. Actually, the width of the front is also substantially affected, featuring fluctuations which again scale as $1/\log N$. Hence, the discrete nature of density fluctuations at a microscopic level induces large, observable randomness at large scales. This implies that there is no weak-noise or deterministic regime in real-life Fisher fronts. Moreover, we have found that the macroscopic front line evolves like a low-pass filter of the edge fluctuations and thus both objects share the same universality class for large spatial and temporal scales. In particular, since the edge is a one-dimensional entity undergoing dynamics which is not constrained by conservations laws [27], we find that front and edge's fluctuations both feature 1D KPZ scaling. Incidentally, kinetic roughening in the KPZ universality class has been recently found in systems for which (stochastic one-dimensional) Fisher-like waves are advocated, such as range expansion of genetically diverse bacterial populations [34,35]. Note that the KPZ behavior that we obtain corresponds to $h_{f,e}$, and not to the variable ρ that satisfies the sFKPP equation (2). It is to be expected that, if one were able to write down the dynamical equation for the effective variables $h_{f,e}$ (which in principle seems a nonstraightforward result for pulled fronts of the sFKPP equation), then the information about the steady-state properties of the KPZ equation could be relevant to their long time behavior. This includes the nonequilibrium potential [36] ensuing in its variational formulation and exact results on KPZ universality [37]. Note that such type of effective equation was actually derived in [26] for other type of noise in the FKPP equation, but our results show that the generalization of this result does not hold in the sFKPP equation (2) where intrinsic fluctuations dominate.

Since stochasticity is inevitable at the edge of 3D traveling waves, our results show that there is no weak-noise or deterministic regime in real-life Fisher fronts. Note that, due to the universality properties that ensue in RD front propagation, one expects Eq. (2) to describe the evolution of a large class of systems, including, e.g., those in the celebrated directed percolation universality class [38], or even to arise in the process of obtaining the normal form for suitable stochastic multiscale systems. This is, in principle, a delicate process in which full separation between fast and slow dynamics can nonetheless be achieved under appropriate conditions [39,40]. Overall, our conclusion on the lack of weak-noise regime in Fisher fronts has an important consequence about the relevance of the deterministic Fisher equation as a model to explain the observations in experimental setups: since Fisher waves are always stochastic, are the observed results affected by a macroscopic noise?

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