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Emergence of pulled fronts in fermionic microscopic particle models

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We study the emergence and dynamics of pulled fronts described by the Fisher-Kolmogorov-Petrovsky-Piscounov (FKPP) equation in the microscopic reaction-diffusion process $A+A\leftrightarrow A$ on the lattice when only a particle is allowed per site. To this end we identify the parameter that controls the strength of internal fluctuations in this model, namely, the number of particles per correlated volume. When internal fluctuations are suppressed, we explictly see the matching between the deterministic FKPP description and the microscopic particle model.

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The study of diffusion-limited reaction processes has shown the important role of internal or microscopic fluctuations in low dimensions [1–3]. Mean-field approximation for those processes assume that diffusive mixing is much stronger than the influence of correlations produced by reactions. However, diffusive mixing is not strong enough in low-dimensional systems and fluctuations might modify the dynamics or induce nonequilibrium phase transitions. While this behavior is observed in different situations, there is an special interest in the problem of front propagation in reaction-diffusion systems [3–17]. In this paper we concentrate in microscopic lattice reaction-diffusion models whose mean-field approximation is given by the Fisher-Kolmogorov-Petrovsky-Piscounov (FKPP) equation [18]

$$\frac{\partial \rho}{\partial t} = D\frac{\partial^2 \rho}{\partial x^2} + k_1\rho - k_2\rho^2, \tag{1}$$

where $\rho(x,t)$ is the local concentration of particles. Such an equation display traveling-wave solutions of the form $\rho=\rho(\xi)$ with $\xi=x-vt$, which invade the unstable phase $\rho=0$ from the stable phase $\rho=k_1/k_2$ and travel with velocity $v\geqslant v_0=2\sqrt{Dk_1}$. For steep enough initial conditions, the solution selected for large times is that with minimal velocity v_0, which is known to be a pulled front, since it is essentially ''pulled along'' by the growth and spreading of small perturbations in the leading edge where $\rho\ll 1$ [4,19]. Microscopic fluctuations are expected to modify macroscopic properties of pulled fronts at two levels: (i) because the deterministic description (1) breaks down at small densities $\rho\sim 1/N$ where N is the number of particles, which introduces an effective cutoff in the FKPP equation; due to the importance of the tail development in pulled fronts, several front features are dramatically affected by this effective cutoff [8], for example, the selected velocity converges as $\ln^{-2}N$ to the mean-field value v_0; (ii) because internal fluctuations are present and could interplay with or even destroy pulled front development and dynamics [5,7,13].

One of the most studied microscopic models is the reversible reaction model $A\leftrightarrow A+A$ on a lattice [5–7,9–17]. In the bosonic version of this model [9], the number of possible particles per site is unbounded and thus the balance between birth and coagulation gives an average number of particles per site N. If $N\to\infty$ the reaction is well stirred within each site and the front dynamics is described by the mean-field approximation (1). For very large N discreteness effects remain and produce the predicted velocity correction $v-v_0\sim\ln^{-2}N$ [8,10]. In the case of the fermionic version of the $A\leftrightarrow A+A$ model only a particle is allowed per site. The main reason to consider exclusion is that, for some values of the parameters, the model is analytically tractable [3,5,7,14] and/or simulations are easier than in the bosonic version. Exact results are available for the two interesting regimes in the model: reaction-limited regime [14], where coarse-grained density front profiles are described by the mean-field FKPP equation, and diffusion-limited regime [3,5,7] in which internal fluctuations dominate front propagation and the mean-field approximation (1) is not valid. Our purpose in this paper is to put these two results in a general framework that can describe the emergence of pulled fronts in this fermionic model. This is done by identifying the control parameter that modulates the effect of internal fluctuations on the front propagation model. As we will see, this parameter also controls the development of the tail front and establishes the appearance of pulled fronts.

In the $A\leftrightarrow A+A$ model in one dimension, particles are allowed to occupy lattice sites and can undergo the following moves: (i) diffusion to any one of its two neighbor lattice sites with a diffusion rate D; (ii) birth, occupied sites spontaneously generate particles at neighbor lattice sites with rate μ; (ii) coagulation, a particle can get annihilated with death rate η if one of its two neighboring filled lattice sites is occupied. The fermionic nature of the model makes diffusion and birth only possible if the neighboring lattice site is empty. The mean-field description of this model is given by the FKPP equation with $k_1=2\mu$, $k_2=2(\mu+\eta)$. Starting from an initial condition in which occupation number is only different from zero on the right side of a site, a front develops and advances as a function of time. Operationally, the front position $x_f(t)$ is determined by a local average of density of particles over intervals of length $\lambda^{-1}=2D/v_0$, which

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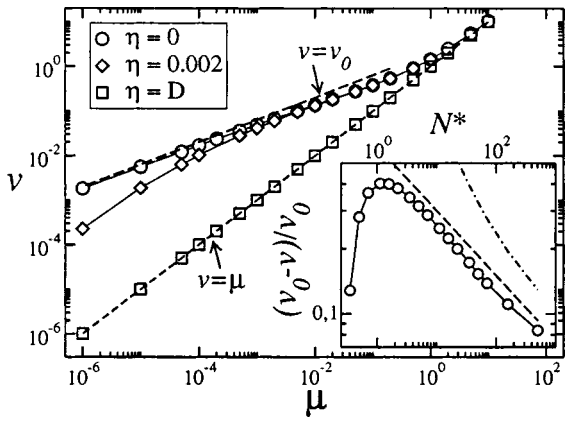

FIG. 1. Velocity as a function of the birth rate μ for different values of the coagulation rate η. Simulations are done with $D=0.5$. Dashed lines correspond to the predictions $v=\mu$ [5,3] and $v=v_0$ [14]. Inset: velocity corrections as a function of N^* for the case $\eta=0$. Dashed line is the power law $N^{-1/3}$ while dash-dotted line is the prediction $\pi^2/(2\ln^2 N^*)$ of Ref. [8].

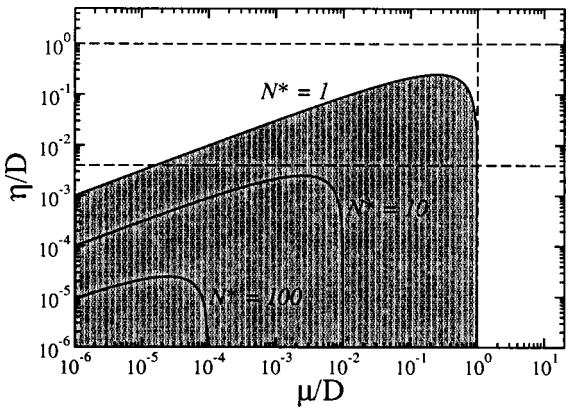

FIG. 2. Schematic diagram of condition (2) in the (η,μ) phase space. Shaded area correspond to those values of the parameters for which $N^*>1$. Solid lines correspond to the solution of Eq. (3) for different values of N^*. Dashed lines are the following sets of parameters: $\eta=D$ [5,7], $\mu=D$ [11], and $\eta=0.002$ used in Fig. 1.

is the width of the deterministic front selected for our initial condition by the FKPP equation (1) [19]. Thus, front position is the point where this coarse-grained density equals $\rho_0/2$ [12,13]. Other definitions of the front position yield the same results [14]. Since results only depend on the ratios D/μ and D/η we set $D=1/2$ throughout this paper. After a transient time (which could be long), the front advances linearly, i.e., $\langle x_f(t)\rangle = vt$, where $\langle\cdots\rangle$ stands for average over different realizations. In this regime, statistical properties of the front with respect to the normalized coordinate $\xi=x-vt$ are independent of time.

In this model, there are two special cases for which exact results are available. When $\eta=D$ the model is solvable using the method of interparticle distribution functions [3,5]. In that case fronts advance with velocity $v=\mu$, which shows how internal fluctuations can dominate the system behavior in this diffusion-limited regime. On the other hand, when $\eta=0$ it was proved in Ref. [14] that fronts approach asymptotically the FKPP equation predictions ($v=v_0$) in the limit $D/\mu\to\infty$ (reaction-limited regime), while $v=D+\mu$ in the opposite regime $D/\mu\to 0$ (diffusion-limited regime). In Fig. 1 we show the results of our simulations for the velocity of the front v as a function of μ for different values of η. Our results are consistent with the exact results [3,5,14] and previous simulations of this model [15]. For an intermediate case $0<\eta<D$ we observe that, for some values of μ, the velocity seems to approach the deterministic value v_0. However, for small enough value of μ internal fluctuations seem to dominate and the velocity deviates strongly from v_0.

To understand this behavior, let us recall that mean-field approximation (1) in the $A\leftrightarrow A+A$ is only valid when diffusive mixing is strong enough. Specifically, this happens when the typical distance traveled diffusively by a particle between reaction events, l_D, is much larger than the typical distance between particles, l_p [3]. In that case, particles are well stirred within cells of size l_D and thus mean-field approximation is valid for the coarse-grained density of particles over cells of size l_D, as shown in Ref. [14]. In our model we have that $l_D=\min(\sqrt{D/\mu},\sqrt{D/\eta})$, while we approximate l_p by the average distance between particles in the stable phase $l_p=\rho_0^{-1}=(\mu+\eta)/\mu$. Since we are interested in the propagation of pulled fronts, which are only driven by the birth term, our condition to approach the mean-field approximation is then given only by μ:

$$\sqrt{D/\mu}\gg\rho_0^{-1}=\frac{\mu+\eta}{\mu}. \tag{2}$$

Interestingly, this condition is equivalent to $N^*\equiv\lambda^{-1}\rho_0\gg 1$, where N^* is approximately the number of particles within an interval of length λ^{-1}. Thus, condition (2) also means that the number of particles within the typical length scale of the front (its width) is large. Our results in Fig. 1 are then easily explained in terms of condition (2): when $N^*\gg 1$ internal fluctuations should be unimportant within cells of size $l_D\simeq\lambda^{-1}$ and front propagation should approach asymptotically the FKPP predictions. Since

$$N^*=\frac{\sqrt{\mu/D}}{\mu/D+\eta/D}, \tag{3}$$

then $N^*\gg 1$ only happens when $(D/\eta)^2\gg D/\mu\gg 1$ for fixed values of D and η. We show the condition $N^*>1$ in Fig. 2 along with the different set of parameters used in Fig. 1 and in other works [5,7,11]. Outside the region $N^*>1$ internal fluctuations dominate and fronts are not described by the FKPP equation. This is the case for $\eta=D$ [3,5] and $\eta=\mu$ [11]. In the intermediate case $0<\eta<D$, we can have values of μ for which N^* is relatively large and fronts seem to approach the deterministic value of v_0, which explains the behavior observed in Fig. 1 for $\eta=0.002$. Note, however, that although being in the region $N^*>1$ is the minimum requirement for our model to approach the mean-field description (1) a finite value of N^* means that fronts are still subject to internal fluctuations and discreteness effects that produce a (strong) correction to the velocity. Only in the

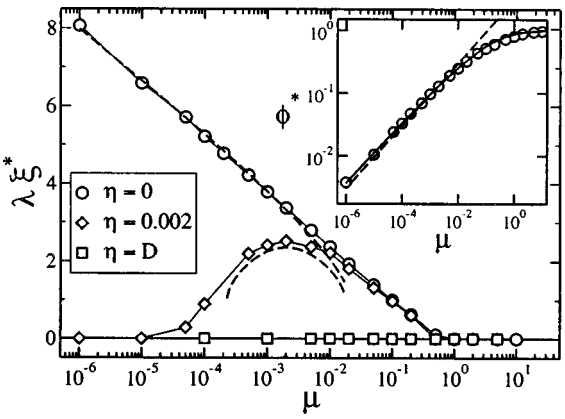

FIG. 3. Position of the last particle from the front position, ξ^*, as a function of μ from simulations. Dashed lines are Eq. (4) with $a=1.4$. Inset: occupation probability for the site just before the last particle (circles). Solid line is given by Eq. (5) with v taken from simulations and dashed line is the approximation $\rho^* \simeq a/\lambda$ used to get Eq. (4) [22].

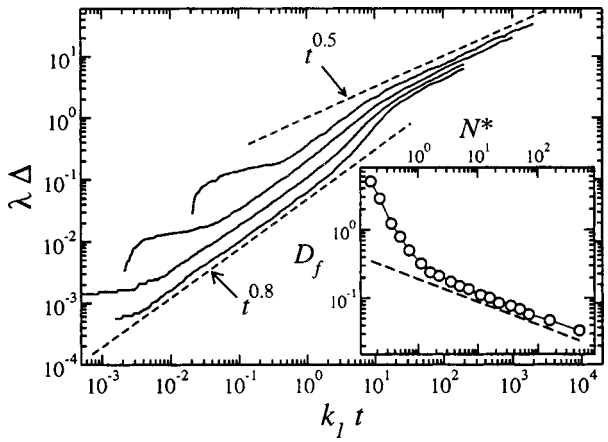

FIG. 4. Time evolution of the diffusive spreading of the front position for different values of μ (solid lines) and $\eta=0$: $\mu = 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}$ from top to bottom. Inset: diffusion coefficient as a function of N^* for $\eta=0$. Dashed line is the power law $(N^*)^{-1/3}$.

limit $N^* \to \infty$ do both effects become negligible and the $A \leftrightarrow A+A$ system is effectively described by the FKPP equation. This is the case for $\eta=0$, $\mu \to 0$ [20].

An interesting question is whether N^* plays any role like the average number of particles per site, N, in bosonic models [8–10]. In those models, it is observed that the deterministic description of a pulled front given by the FKPP equation is valid until the density drops to $\rho \simeq N^{-1}$, which produces an effective cutoff in the tail of the front and modifies its velocity [8]. To check this possibility, we have measured in our simulations the average distance of the last particle from the front position, ξ^*, which is observed to saturate to a constant value for long enough times. It is obvious that for $\xi > \xi^*$ the continuum description of the front breaks down and we expect this to happen when there is only a particle in each coarse-grained site of length λ^{-1}, i.e., when $\rho(\xi^*) \simeq a\lambda$, where a is a constant. When internal fluctuations are irrelevant, i.e. when $N^* \gg 1$, we assume that continuum description (1) is still valid up to ξ^* and taking that $\rho \simeq \rho_0 \lambda \xi e^{-\lambda \xi}$ for $\lambda \xi \geqslant 1$ for a pulled front [19] we obtain

$$\lambda \xi^* e^{-\lambda \xi^*} = a/N^*. \tag{4}$$

Solutions of this equation for ξ^* with N^* given by Eq. (3) are compared with our simulations in Fig. 3. We see that for $\lambda \xi^* \gtrsim 1$ Eq. (4) gives a rather accurate prediction of ξ^*. This corroborates our assumption that a pulled front described by the FKPP equation develops even for moderate values of N^* up to the point where $\rho \simeq (N^*)^{-1}$.

An important consequence of Eq. (4) is that N^* controls not only the size of internal fluctuations but also the appearance and length of the tail in the pulled front. Thus, when $N^* \lesssim 1$ internal fluctuations dominate and also the tail length is roughly zero, $\lambda \xi^* \simeq 0$. This means that the front is basically a shock wave with height ρ_0. Actually, the exact solution when $\eta = D$ [7] shows that the particles behind the leading one remain distributed as in the stable phase ($\rho = \rho_0$) at all times, which confirm our picture (see Fig. 3). This *shock wave* shape is also observed in the case $\eta \neq D$ when $\mu \gg \eta$, where it is found that $\lambda \xi \simeq 0$. In the intermediate case in which $\eta \neq 0$, we see that the front develops a tail, which is described by the FKPP equation only for a given interval of values of μ (see Fig. 3 for $\eta = 0.002$).

In the case $\eta=0$ we have studied the correction to the velocity as a function of N^* and observe in the inset of Fig. 1 that it decays like $(v_0 - v)/v_0 \sim (N^*)^{-1/3}$, which is consistent with simulations of other microscopic bosonic models [8,17] for moderate values of number of particles N. This result stresses the equivalence of N^* with the role that the number of particles plays in other microscopic models. In particular we expect the correction to be $(v - v_0)/v_0 \sim \ln^{-2} N^*$ for very large values of N^* [21].

Since the last particle is, on average, at a certain distance from the front position, their velocities coincide. This fact was used in Refs. [11,15] to estimate the velocity of the front by counting possible forward and backward hopping rates:

$$v = \mu - \rho^*(\eta - D), \tag{5}$$

where ρ^* is the probability of having a particle behind the last one. Several approximations can be made for the value of ρ^* [11,15]. For example, in Ref. [11] it was taken as $\rho^* \simeq \rho_0$, i.e., ρ^* is given by the probability to find a particle in the stable phase. Clearly, this approximation is only valid in the case in which fronts are like a shock wave, i.e., when $N^* \simeq 1$ because then the last particle is very close to the stable phase. In the case in which a pulled front develops ($N^* \gg 1$) we find that Eq. (5) still holds; since the last particle is on average at a fixed distance from the front position, we can approximate $\rho^* \sim \rho_0 \lambda \xi^* e^{-\lambda \xi^*} = a/\lambda$, which is the concentration of particles at ξ^*. Our simulations for $\eta=0$ confirm the validity of this approximation (see Fig. 3) which brings out the effective matching between the continuum description given by the FKPP equation for $\xi < \xi^*$ and the microscopic character of the model for $\xi \gtrsim \xi^*$.

Another interesting property of front propagation is the wandering of the position of the front around its mean value $\Delta^2(t)=\langle[x_f(t)-\langle x_f(t)\rangle]^2\rangle$. Several studies of different microscopic models show that $\Delta^2(t)=2D_f t$ for long times [8,9,17] and that the diffusion coefficient D_f depends on the number of particles N. Specifically, it was found that $D_f \sim N^{-1/3}$ for moderate values of N [9,17], while $D_f \sim \ln^{-3} N$ for very large values of N [8]. Our simulations for the $A+A\leftrightarrow A$ system shows that fronts move diffusively for all values of the parameters. In the case $\eta=0$, in which the model approaches asymptotically the FKPP equation, we get $D_f \sim (N^*)^{-1/3}$ (see Fig. 4) like in bosonic models [17] that stress once again the fact that N^* plays the role of the number of particles in this fermionic model. Moreover, we found for small times that as N^* increases, the correlation between the time development of the front and internal fluctuations produces superdiffusive motion of the front position $\Delta^2(t) \sim t^{2\nu}$ with $\nu \simeq 0.8$. Once the front tail is developed (which happens at $t \simeq k_1^{-1}$), the front position starts to wander diffusively. Finally, our results for the diffusion of the front indicate that as the front approaches the deterministic FKPP equation, internal fluctuations make the front move diffusively at times $t > k_1^{-1}$, independent of N^*. We do not observe any signs of subdiffusive behavior in the limit N^* to ∞ conjectured by some authors [4,12] for pulled fronts subject to noise. This supports the idea that pulled fronts subject to internal noise belong to a different universality class than those subject to external noise [13].

In summary, we have identified the parameter that controls the strength of microscopic fluctuations for the front propagation problem in the fermionic model $A\leftrightarrow A+A$, namely, the number of particles N^* per coarse-grained site of length λ^{-1}. When $N^* \gg 1$, internal fluctuations are suppressed and the front becomes a pulled front like those of the FKPP equation (1). Moreover, our studies about the length of the tail, the velocity of the front, and its diffusion show that N^* plays the same role as the number of particles in other microscopic bosonic models. Finally, it is interesting to note that in the $A\leftrightarrow A+A$ model, the velocity of a macroscopic object such as the front is related to the microscopic motion of the last particle, something also observed in other works [8,11,16]. We hope our results will help understand the dynamics of fronts in microscopic fermionic reaction-diffusion models and its relevance when discussing properties of the FKPP equation subject to internal noise [4,12,13].

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[20] Note, however, that other scalings like $\eta \sim \mu$ in Eq. (3) are possible to get $N^* \to \infty$ in the limit $\mu \to 0$.
[21] A crude estimation for this to happen is when $N^{-1/3} \simeq \pi^2/(2 \ln^2 N^*)$ [8], which gives $N^* \sim 10^4$, beyond our range of values for N^*.
[22] Due to the coarse-graining over intervals of length λ^{-1} to calculate the front position, ξ^* could be negative. In that case we take $\xi^*=0$ since it is obvious that the last particle is the one that defines the front position.