

Rare Events in Stochastic Partial Differential Equations on Large Spatial Domains

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Abstract A methodology is proposed for studying rare events in stochastic partial differential equations in systems that are so large that standard large deviation theory does not apply. The idea is to deduce the behavior of the original model by breaking the system into appropriately scaled subsystems that are sufficiently small for large deviation theory to apply but sufficiently large to be asymptotically independent from one another. The methodology is illustrated in the context of a simple one-dimensional stochastic partial differential equation. The application reveals a connection between the dynamics of the partial differential equation and the classical Johnson–Mehl–Avrami–Kolmogorov nucleation and growth model. It also illustrates that rare events are much more likely and predictable in large systems than in small ones due to the extra entropy provided by space.

Keywords Rare events · Metastability · Nucleation · Phase transformation · Small noise · Large deviation theory · Spatially extended system · Stochastic partial differential equation

1 Introduction

This paper is motivated by the physical problem of metastability and phase separation, and an interest in quantifying the effects of nucleation and growth in stochastically perturbed reaction diffusion systems. Familiar examples of metastability include the condensation of supercooled vapor and the phase separation of a binary alloy; for a nice discussion and experimental pictures see for instance [27, 40]. In contrast to spinodal decomposition, in which a system evolves from a deterministically *unstable* state towards an energy minimum, metastability refers to a system that starts in a deterministically *stable* state and evolves, due

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to thermal noise, towards the global energy minimum. Put differently, metastability involves crossing an energy barrier. Because the timescale for crossing the energy barrier is typically large, the initial state of the system persists for a long time; hence the name metastable.

The size of the system is critical in determining the pathway of a metastable system. It is well known that in small systems, a *single droplet pathway* dominates; many small droplets form and disappear until eventually a large fluctuation leads to the formation of one so-called critical droplet or critical nucleus which then grows to take over the system. However it is in large systems that the spatial extent of the system comes into play and a *multiple droplet pathway* dominates [46, 50]. Nucleation and growth in physical systems typically resembles the multiple droplet regime [27, 40].

Mathematically, there are two main branches of the study of stochastic metastability: the microscopic approach that studies spin systems and the macroscopic approach that studies stochastically perturbed differential equations. Significant progress has been made in the microscopic branch: The multiple droplet regime of metastability has been analyzed in [16, 47, 48]; see also [18, 19, 25] for analysis of nontrivial spatial structure in the case of relaxation from a deterministically unstable state.

In contrast, in the macroscopic branch the multiple droplet regime is yet to be investigated. Before going further, let us introduce the macroscopic model on which we will focus; see also Remark 1.

1.1 A Ginzburg–Landau Model

The simplest macroscopic model is the “Model A” reaction diffusion equation

$$\dot{u} = u_{xx} - V'(u), \quad (1.1)$$

where $u : [0, T] \times [-L, L] \rightarrow \mathbb{R}$ is the scalar order parameter, \dot{u} represents the time derivative of u , and V is a double-well potential with minima $u_- < u_+$. Notice that “Model A” does not conserve the order parameter, in contrast to “Model B,” according to the classification of Halperin and Hohenberg [28]; see also Remark 1 below. The stochastically perturbed version of (1.1) is

$$\dot{u} = u_{xx} - V'(u) + \sqrt{2\varepsilon}\eta, \quad (1.2)$$

where η is a space-time white noise and ε is the noise intensity, the inverse of the dimensionless temperature.

Reaction diffusion equations such as (1.1) have been obtained as limits of microscopic models [6, 17]. They have also been used broadly as phenomenological models, including for instance to model chemical reactions, population dynamics, and wave propagation [20]. Qualitatively, the salient feature of (1.1) is that it is the gradient flow (with respect to L^2) of the Ginzburg–Landau energy

$$\int_{-L}^L \left(\frac{1}{2} u_x^2 + V(u) \right) dx. \quad (1.3)$$

Therefore solutions tend toward minima of (1.3), which prefer to be constant in space (to keep gradients small) and prefer to take values u_- and u_+ (to minimize the bulk energy from $V(\cdot)$). If boundary conditions permit, the unique energy minimizers are the functions $u \equiv u_-$ and $u \equiv u_+$.

The well-known Allen Cahn equation is (1.1) with a *symmetric* potential, often written as

$$V_0(u) = \frac{1}{4}(1 - u^2)^2.$$

However we will be mainly concerned with the case of an *asymmetric* potential. Asymmetric potentials arise for instance when there is an external field:

$$V(u) = V_0(u) - hu.$$

In this case $u \equiv u_-$ is a *local* energy minimizer, but the unique *global* energy minimizer is $u \equiv u_+$. We note for future reference that the deterministic PDE with unequal well potential has a “critical nucleus” even in an infinite system, which means, roughly speaking, that the $L \rightarrow \infty$ limit of the diameter of the lowest-energy saddle point exists. (Strictly speaking, in the Allen Cahn equation there is no critical nucleus in an unbounded system since the diameter of the lowest-energy saddle point becomes infinite as $L \rightarrow \infty$.)

The stochastic term in (1.2) reflects small scale noise that perturbs the deterministic dynamics. The noise gives rise to metastability: If the system starts at the local energy minimizer $u(0, \cdot) = u_-$, then the solution will exhibit small fluctuations around this state until a large deviation drives the system over the energy barrier and into a small neighborhood of the global minimizer $u \equiv u_+$. (In any bounded system the solution will eventually switch *back* to a neighborhood of the local minimizer, but since the expected lifetime near the global minimizer is exponentially longer than that near the local minimizer, the local minimizer is referred to as the metastable state and the global minimizer is often called, somewhat misleadingly, the stable state.)

1.2 Metastability in Stochastic PDE

The celebrated large deviation theory of Freidlin and Wentzell [23] provides a rigorous mathematical analysis of metastability in finite dimensional (ODE) systems. Freidlin–Wentzell theory generalizes naturally to infinite dimensional (PDE) systems. The classic paper [22] analyzes metastability in the stochastically perturbed Allen Cahn equation. Another important paper is [38], which analyzes the expected value of the time to switch from one energy minimizer to a neighborhood of the other and proves that, on this timescale, the exit probability is exponentially distributed in time. See also [14, 15] for general theory in infinite dimensions.

All of these results, however, concern the “single droplet” regime of stochastic PDE. More precisely, (1.2) is studied on the fixed space domain $[-L, L]$ in the zero noise limit: $\varepsilon \rightarrow 0$. Very little is known about (1.2) on the space domain $[-L_\varepsilon, L_\varepsilon]$ in the limit with $L_\varepsilon \rightarrow \infty$ as $\varepsilon \rightarrow 0$. One extension is [12], in which it is shown that for (1.2) with an asymmetric potential, as long as L_ε does not grow too quickly as $\varepsilon \rightarrow 0$, the single droplet picture of Freidlin–Wentzell theory is preserved.

The multiple droplet regime of (1.2) is precisely the regime in which L_ε grows sufficiently quickly as $\varepsilon \rightarrow 0$. One result that is independent of the system size is [45], in which it is shown that the invariant measure of (1.2) with Dirichlet boundary conditions is equivalent to the law of a bridge process with a modified potential. For small noise, it suggests that in the case of an asymmetric potential with $V(u_-) > V(u_+)$, the invariant measure will be supported on functions $u \approx u_+$. What about the metastable *dynamics*? The intuition is that in a large system, the sheer number of possible nucleation locations should be important. Indeed, although a nucleation event is exponentially unlikely with respect to ε^{-1} , if the

system is exponentially large with respect to ε^{-1} , then finding a nucleation somewhere in the system is likely. As a result, rather than being dominated by a single most likely pathway, phase transformation is most likely to occur via multiple nucleations that are randomly distributed in space and time.

A fundamental question is: How can we derive the distribution of the multiple, random nucleation events in the large system setting? There are also properties of the transformation that we would like to quantify and understand. For instance, one expects the multiple nucleations to lead to a transformation time-scale (e.g., the time for an n th of the system to be transformed) that is much shorter than if the transformation were generated by a single nucleation. Moreover, in the large system limit, *deterministic properties* should emerge: Each nucleation is a rare event, but the net behavior is governed by the law of large numbers.

In this paper, we suggest a framework to study rare events in large systems by considering subsystems that are small enough so that prefactor estimates for the mean nucleation time can be derived, but large enough that the behavior on different subsystems is asymptotically independent. To derive reduced dynamics, the dynamics of the deterministic PDE (1.1) will be important. We study the case of an asymmetric potential precisely because—in addition to yielding a critical radius—the deterministic dynamics following the formation of a critical droplet is simple. Indeed, interfaces connecting $u \approx u_-$ and $u \approx u_+$ are formed which then spread with a *finite* travelling wave velocity [8]. See also Remark 2 below.

Our method will require an estimate—including the prefactor—for the nucleation rate $\Lambda_{\ell_\varepsilon}^{\ell_\varepsilon}$ on a subsystem of scale ℓ_ε with $\ell_\varepsilon \gg \ln \varepsilon^{-1}$. This is a question of independent interest. Prefactor estimates have been well studied (see for instance [7, 32–34, 36, 39, 49] and the references therein), but the usual estimate breaks down in our scaling. The entropic effect of the subsystem size leads to an ℓ_ε dependence in the prefactor:

$$\Lambda_{\ell_\varepsilon}^{\ell_\varepsilon} \propto \ell_\varepsilon \varepsilon^{-1/2} \exp(-\Delta E^{\ell_\varepsilon} / \varepsilon), \quad (1.4)$$

where $\Delta E^{\ell_\varepsilon}$ denotes the energy barrier for the subsystem. The scaling in (1.4) has been observed before [10, 26, 34, 35, 39]; we give a new derivation using formal asymptotics and the Co-area Formula. (See Sect. 2.2 for details.) Estimating $\Lambda_{\ell_\varepsilon}^{\ell_\varepsilon}$ represents an infinite-dimensional version of a degenerate escape rate problem, i.e., estimating the escape rate for a particle out of a potential well for which the saddle point is not an isolated point. Recently *capacities* have proven useful in the analysis of escape rate problems [7, 21]. Although prefactor estimates for *nondegenerate* potentials in the *finite dimensional* case have only recently been proven rigorously in [7], the method of capacities used there seems natural for an extension to infinite dimensions.

In Sect. 2 we review the rate problem and its long history, and derive the generalization (2.7), (2.8). Then in Sect. 3, we apply the nucleation rate estimate to study phase transformation in (1.2). Taking appropriate limits, we reduce the spatially-distributed phase transformation to a simple version of the Johnson–Mehl–Avrami–Kolmogorov (JMAK) model [4, 11, 30, 31]. Here, the new contribution is the connection between the SPDE and the JMAK model which, as we explain, allows one to observe and quantify the drastically reduced transformation time-scale and the deterministic limiting behavior that emerge for large systems.

Remark 1 Of course, in addition to (1.1) there are many other physically relevant and mathematically interesting models. In higher space dimensions, the Allen Cahn equation

$$\dot{u} = \Delta u - V'_0(u)$$

is a phase field approximation of motion of interfaces by mean curvature. The fourth order Cahn Hilliard equation

$$\dot{u} = -\Delta(\Delta u - V'_0(u))$$

conserves the mean value of the order parameter (a ‘‘Model B’’ equation). In this paper we focus on one example. Equation (1.1) with an *asymmetric* double-well potential is simple enough to allow a thorough analysis: The asymmetry leads to (1) a critical droplet size and (2) the deterministic spreading of the new phase once a critical droplet has formed. The framework we propose, however, is more general and may be applied to other models.

Remark 2 The dynamics of kink motion in the stochastic Allen Cahn equation (symmetric potential) is analyzed in [9, 24]. It is proved that in the sharp interface limit, the dynamics of a kink reduces to the diffusive motion of a single point. One would also like to understand rare events in the Allen Cahn equation, i.e., given initial data $u \equiv -1$, how do kinks form? However even the limit picture is not clear. Kinks should reduce to diffusive points that annihilate upon collision, but Brownian motions started at the same point cross infinitely often before separating. The nonzero drift in the case of the asymmetric potential makes that case easier.

2 Escape Rate in Degenerate Potentials

The study of the rate of escape from a stable state goes back to Arrhenius [3] for the chemical reaction rate. In the nondegenerate case—i.e., the case in which one considers escape from an isolated minimum of the potential, there is a unique energy-minimizing saddle point on the boundary of its basin of attraction, and the Hessians of the energy at the minimum and the saddle point have no zero eigenvalue—the problem was analyzed for $d = 1$ in [32] and $d > 1$ in [33, 36, 39, 49]. Recently, the rate estimate was derived as a mathematically rigorous result in [7]. For the nondegenerate, infinite-dimensional case, we refer the reader to [14, 15, 38].

We are interested in the case that is *degenerate* in the sense that the minimum of V on the boundary ∂D is not an isolated point. Estimates for the escape rate in the degenerate case were introduced as early as [26], and have been developed in [10, 34, 35, 39]. The most important difference from the estimate in the nondegenerate case is the appearance of an extra volume factor, the volume of the subspace corresponding to the degenerate saddle point. In this section, we give a new derivation of the escape rate in the degenerate case in order to obtain (2.7) and (2.8), which reduce to the estimates in [34, 35] under simplifying assumptions (cf. Remark 3). We consider the finite dimensional case in Sect. 2.1 and then interpret our result in the infinite dimensional setting in Sect. 2.2.

2.1 Finite Dimensional Setting

We consider the stochastically perturbed gradient flow

$$dX_t = -\nabla V(X_t) dt + \sqrt{2\varepsilon} dW_t, \quad X_0 = x, \tag{2.1}$$

where $W_t \in \mathbb{R}^N$ is an N -dimensional Brownian motion. We suppose that $V : \mathbb{R}^N \rightarrow \mathbb{R}$ is a potential with an isolated, nondegenerate minimum at x_m . We denote by D the basin of attraction of x_m , i.e.

$$D = \{x \mid \lim_{t \rightarrow \infty} z(t) = x_m \text{ where } \dot{z} = -\nabla V(z) \text{ with } z(0) = x\}, \tag{2.2}$$

and we wish to analyze the problem of first exit out of D by the process defined in (2.1). More precisely, we wish to analyze the properties of the first exit time

$$\tau_\varepsilon(x) = \inf\{t \mid X_t \notin D, X_0 = x \in D\}. \tag{2.3}$$

As $\varepsilon \rightarrow 0$, the escape from D can be represented asymptotically as a Poisson process with intensity Λ_ε :

$$\lim_{\varepsilon \rightarrow 0} \mathbb{P}(\Lambda_\varepsilon \tau_\varepsilon(x) \geq s > 0) = e^{-s} \quad \text{for any } x \in D, \tag{2.4}$$

where

$$\Lambda_\varepsilon = \sqrt{\frac{\varepsilon}{2\pi}} \frac{\int_{\partial D} |\langle \hat{n}(x), H(x)\hat{n}(x) \rangle|^{1/2} \exp(-V(x)/\varepsilon) d\sigma}{\int_D \exp(-V(x)/\varepsilon) dx}. \tag{2.5}$$

Here $H(x)$ is the Hessian of $V(x)$, $\hat{n}(x)$ denotes the outward normal to ∂D at point $x \in \partial D$, and $d\sigma$ is the surface measure on ∂D . Equations (2.4) and (2.5) can be derived by formal asymptotics [36]. (See also the Appendix B of [2]. They consider the nongradient case and derive a more general formula that reduces to (2.5) in the gradient case (2.1).) A rigorous derivation of (2.4) for Λ_ε of the correct exponential order has been given in [38].

For a nondegenerate potential, the main contribution to the integral in the denominator of (2.5) comes from the point $x_m \in D$ where V is minimized, and the main contribution to the integral in the numerator comes from the point of minimum energy on ∂D (i.e., the lowest energy saddle point). Expanding V to second order around the respective critical points leads to

$$\Lambda_\varepsilon = (C + o(1)_{\varepsilon \rightarrow 0}) \exp(-\Delta V/\varepsilon) \quad \text{with} \quad C = \frac{1}{2\pi} \sqrt{|\lambda_1^s| \lambda_1^m} \prod_{j=2}^N \sqrt{\frac{\lambda_j^m}{\lambda_j^s}}, \tag{2.6}$$

where λ_j^s and λ_j^m are the eigenvalues of the Hessian of the energy at the saddle and minimum, arranged in ascending order. This is called the harmonic expansion. Note that the factor $|\langle \hat{n}(x), H(x)\hat{n}(x) \rangle|$ contributes $|\lambda_1^s|$, the magnitude of the unique negative eigenvalue of the Hessian at the saddle point.

When the potential is degenerate, the harmonic expansion leading to (2.6) is not valid. Suppose that instead of being peaked at a single point on ∂D , $\exp(-V/\varepsilon)$ is peaked at a continuum of energy-minimizing saddle points

$$S := \operatorname{argmin}_{x \in \partial D} V(x),$$

all of which contribute to the denominator in (2.5). We assume for simplicity that S is a manifold without boundary, and parameterize the set as

$$S = \{\gamma(\theta); \theta \in [0, 1]^d\}.$$

We claim that in this case, (2.5) can be reduced to

$$\Lambda_\varepsilon = (\bar{C}_\varepsilon + o(\varepsilon^{-d/2})) \exp(-\Delta V/\varepsilon), \tag{2.7}$$

where

$$\bar{C}_\varepsilon = \frac{1}{2\pi} (2\pi\varepsilon)^{-d/2} \int_{[0,1]^d} J(\theta) \sqrt{|\lambda_1^s(\theta)|} \prod_{j=1}^{d+1} \sqrt{\lambda_j^m} \prod_{j=d+2}^N \sqrt{\frac{\lambda_j^m}{\lambda_j^s(\theta)}} d\theta. \tag{2.8}$$

Here $J(\theta)$ is the Jacobian defined as

$$J(\theta) = \sqrt{\det(\nabla\gamma(\theta)(\nabla\gamma(\theta))^T)}, \tag{2.9}$$

$\lambda_j^s(\theta)$ represent the eigenvalues of $H^s(\gamma(\theta))$ (the Hessian of V at $\gamma(\theta)$), and as before λ_j^m represent the eigenvalues of H^m (the Hessian of V at the minimum x_m). We remark that

$$\lambda_1^s(\theta) < 0 = \lambda_2^s(\theta) = \lambda_3^s(\theta) = \dots = \lambda_{d+1}^s(\theta) < \lambda_{d+2}^s(\theta) \leq \dots \leq \lambda_N^s(\theta),$$

so that in particular, 0 is an eigenvalue with multiplicity $d \geq 1$, the dimension of S .

We now derive (2.7) and (2.8) from (2.5).

Step 1. We begin by noticing that (2.5) is equivalent to

$$\Lambda_\varepsilon = (\bar{C}_\varepsilon + o(\varepsilon^{-d/2})) \exp(-\Delta V/\varepsilon),$$

where

$$\bar{C}_\varepsilon = \frac{1}{2\pi} \frac{\int_{\mathbb{R}^N} \exp(-\frac{1}{2\varepsilon} \langle x - Px, H_*^s(Px)(x - Px) \rangle) dx}{\int_{\mathbb{R}^N} \exp(-\frac{1}{2\varepsilon} \langle x, H^m x \rangle) dx}. \tag{2.10}$$

Here the projection $Px = \gamma(\theta_*)$ is defined via

$$\theta_* := \operatorname{argmin}_{\theta \in [0,1]^d} \operatorname{dist}(x, \gamma(\theta)),$$

and the convexification H_*^s is given by

$$\langle x, H_*^s(\gamma(\theta))x \rangle = \langle x, H^s(\gamma(\theta))x \rangle + \frac{1}{2} \left(|\lambda_1^s| + \frac{1}{|\lambda_1^s|} \right) \langle x, v_1^s(\theta) \rangle^2, \tag{2.11}$$

where $v_1^s(\theta)$ represents the eigenvalue of $H^s(\gamma(\theta))$ corresponding to $\lambda_1^s(\theta) < 0$. (Notice that H_*^s is not *strictly* convex because of the zero eigenvalue.)

To see this, notice that in the denominator of (2.5), we have used the standard harmonic approximation. In the numerator, on the other hand, we have observed that the dominant contribution comes from points in ∂D within a small neighborhood of γ . Therefore we expand locally around each point in γ , with the curvature of ∂D contributing only at higher order. At the same time, we “add a dimension” and absorb the factor of $|\langle \hat{n}(x), H(x)\hat{n}(x) \rangle|^{1/2}$ by convexifying H^s as in (2.11) and expanding in the direction perpendicular to ∂D . Finally, as usual the leading order factor is unchanged when we enlarge from a small neighborhood of γ to all of \mathbb{R}^N .

Step 2. Now we remark that (2.10) can be reduced to (2.8). Indeed, the Gaussian integral in the denominator of (2.10) can be evaluated explicitly:

$$\int_{\mathbb{R}^N} \exp\left(-\frac{1}{2\varepsilon} \langle x, H^m x \rangle\right) dx = \frac{(2\pi\varepsilon)^{N/2}}{\prod_{j=1}^N (\lambda_j^m)^{1/2}}. \tag{2.12}$$

The integral in the numerator, on the other hand, can be estimated using once again that only the integration in a neighborhood of $\gamma(\theta)$ contributes at leading order and applying the

Co-area Formula to evaluate the contribution. This gives:

$$\begin{aligned}
 & \lim_{\varepsilon \rightarrow 0} \varepsilon^{(d-N)/2} \int_{\mathbb{R}^N} \exp\left(-\frac{1}{2\varepsilon} \langle x - Px, H_*^s(Px)(x - Px) \rangle\right) dx \\
 &= \lim_{\varepsilon \rightarrow 0} \varepsilon^{(d-N)/2} \int_{[0,1]^d} \int_{\{Px=\gamma(\theta)\}} J(\theta) \\
 & \quad \times \exp\left(-\frac{1}{2\varepsilon} \langle x - \gamma(\theta), H_*^s(\gamma(\theta))(x - \gamma(\theta)) \rangle\right) d\mathcal{H}^{N-d} d\theta \\
 &= \int_{[0,1]^d} J(\theta) (2\pi)^{(N-d)/2} \frac{|\lambda_1^s(\theta)|^{1/2}}{\prod_{j=d+2}^N (\lambda_j^s(\theta))^{1/2}} d\theta. \tag{2.13}
 \end{aligned}$$

Remark 3 In the particularly simple case with $d = 1$ and λ_j^s independent of θ , (2.8) becomes

$$\bar{C}_\varepsilon = \frac{1}{2\pi} (2\pi\varepsilon)^{-1/2} (|\lambda_1^s| \lambda_1^m \lambda_2^m)^{1/2} \prod_{j=3}^N (\lambda_j^m / \lambda_j^s)^{1/2} \int_0^1 \|\gamma'(\theta)\| d\theta, \tag{2.14}$$

which agrees with [34, 35], and which will be relevant for us in the case of the SPDE (1.2).

Remark 4 Our assumptions on S can be relaxed. For instance, our arguments also apply when $H^s = H_\varepsilon^s$ has no zero eigenvalue, but has a small eigenvalue $\lambda_{1,\varepsilon}^s$ that goes to zero so quickly as $\varepsilon \rightarrow 0$ that the harmonic approximation (2.6) breaks down. Then the saddle point is isolated, but because the energy landscape is flat *in the limit*, the contribution of neighboring points must also be taken into account. Although this example may seem contrived, it will be relevant when we consider the SPDE (1.2). See Remark 5 for more.

2.2 Infinite Dimensional Setting

As mentioned earlier, (2.4) has been justified rigorously for $N = \infty$ in the nondegenerate case, with a rate Λ_ε of the correct exponential order [38]. We work under the assumption that (2.4) remains valid with Λ_ε given by (2.6) for $N = \infty$ in the nondegenerate case and by (2.8) for $N = \infty$ in the degenerate case. This can be justified formally by interpreting (2.5) in terms of functional integrals and proceeding as in Sect. 2.1. See also Remark 6.

Consider (1.2) for $x \in [-\ell_\varepsilon/2, \ell_\varepsilon/2]$ with periodic boundary conditions. (Dirichlet boundary conditions are discussed in Remark 5.) Recall that η is a space-time white noise and V is an asymmetric double-well potential. Assume that the minima u_- and u_+ are such that $V(u_-) > V(u_+)$. Suppose that initially, $u(\cdot, 0) = u_-$. An energy barrier separates this state from the absolute minimizer $u(\cdot) = u_+$. We are interested in the mean time to exit the basin of attraction $D(u_-)$ of the initial state.

Let $u_s(\cdot)$ denote a saddle point of least energy. It is a nonconstant, periodic solution of

$$-u_{xx} + V'(u) = 0 \tag{2.15}$$

with minimal energy. Because of the periodic boundary conditions, there is not a unique energy-minimizing saddle point, but rather a one-parameter family:

$$S := \{w(\theta) := u_s(\cdot - \theta), \theta \in [-\ell_\varepsilon/2, \ell_\varepsilon/2]\}.$$

The eigenfunctions $\phi_k^s(\cdot - \theta)$ of the Hessian $H^s(w(\theta))$ solve

$$-\partial_{xx}\phi_k^s + V''(w(\theta))\phi_k^s = \lambda_k^s,$$

and can be chosen orthonormal with respect to the L^2 inner product, i.e.,

$$\langle \phi_j^s(\cdot - \theta), \phi_k^s(\cdot - \theta) \rangle := \int_0^{\ell_\varepsilon} \phi_j^s(x - \theta)\phi_k^s(x - \theta) dx = \delta_{j,k}.$$

Notice that the corresponding eigenvalues

$$\lambda_1^s < 0 = \lambda_2^s < \lambda_3^s \leq \dots$$

are independent of θ . Moreover, it follows in the usual way that

$$\phi_2^s(\cdot - \theta) = \frac{w'(\theta)}{\|w'(\theta)\|_{L^2((-\ell_\varepsilon/2, \ell_\varepsilon/2))}}.$$

In this case (2.7) and (2.14) become

$$\Lambda_\varepsilon^{\ell_\varepsilon} = (C_\varepsilon^{\ell_\varepsilon} + o(\varepsilon^{-1/2})) \exp(-\Delta E^{\ell_\varepsilon} / \varepsilon) \tag{2.16}$$

with

$$\begin{aligned} C_\varepsilon^{\ell_\varepsilon} &= \frac{1}{2\pi} (2\pi\varepsilon)^{-1/2} (|\lambda_1^s| \lambda_1^m \lambda_2^m)^{1/2} \prod_{j=3}^\infty (\lambda_j^m / \lambda_j^s)^{1/2} \int_0^{\ell_\varepsilon} \|w'(\theta)\|_{L^2((-\ell_\varepsilon/2, \ell_\varepsilon/2))} d\theta \\ &= \frac{1}{2\pi} (2\pi\varepsilon)^{-1/2} (|\lambda_1^s| \lambda_1^m \lambda_2^m)^{1/2} \prod_{j=3}^\infty (\lambda_j^m / \lambda_j^s)^{1/2} \ell_\varepsilon \|u'_s\|_{L^2((-\ell_\varepsilon/2, \ell_\varepsilon/2))}. \end{aligned} \tag{2.17}$$

For the convergence of the infinite product, we refer the reader to [37, 43, 44].

Remark 5 The same result holds for (1.2) subject to Dirichlet boundary conditions when the system size satisfies

$$\ell_\varepsilon \gg \ln \varepsilon^{-1}. \tag{2.18}$$

Although in this case for any $\varepsilon > 0$ there is a unique energy-minimizing saddle point, the harmonic approximation is valid only if

$$\frac{\lambda_{\min}}{\varepsilon} \gg 1 \quad \text{as } \varepsilon \rightarrow 0, \tag{2.19}$$

where λ_{\min} is the smallest positive eigenvalue of the Hessian at the saddle point. It is well-known that λ_{\min} is exponentially small with respect to ℓ_ε ; hence, (2.19) is violated in the case of (2.18).

Remark 6 In the nondegenerate case, (2.6) can be derived by interpreting (2.5) as an appropriate expectation with respect to a Gaussian process (or a ratio of partition functions) and applying the results from [14]. Formally, (2.16) and (2.17) can be derived from (2.5) in the infinite-dimensional degenerate case in a similar way, as a product of expectations. Using expectations with respect to infinite dimensional Gaussian processes in order to estimate the nucleation rate may provide an interesting alternative to function space integrals.

3 Metastability in the SPDE Model

Consider stochastically-driven phase transformation in (1.2) with $u(\cdot, 0) = u_-$. We will use the term “nucleation” to mean passing through a critical nucleus (a least energy saddle point, see (2.15)) and exiting the domain of attraction of u_- . For a fixed system size ℓ and $\varepsilon \rightarrow 0$, (1.2) satisfies the exponential law (2.4) with nucleation rate

$$\Lambda_\varepsilon = (C + o(1)_{\varepsilon \rightarrow 0}) \exp(-\Delta E^\ell / \varepsilon), \quad C = \frac{1}{2\pi} \sqrt{|\lambda_1^s| |\lambda_1^m|} \prod_{j=2}^\infty \sqrt{\frac{\lambda_j^m}{\lambda_j^s}}.$$

When the system size L_ε grows quickly as $\varepsilon \rightarrow 0$, on the other hand, there is a competition between the small size of the noise—meaning that nucleation is unlikely—and the large size of the system—meaning that there are many possible places at which nucleation could occur.

The asymmetry of the potential is important: Because of it, minimum-energy saddle points on $[-\ell/2, \ell/2]$ have a “critical radius” that converges to a finite limit as $\ell \rightarrow \infty$. Moreover, there is a deterministic mechanism driving the spread of u_+ : Traveling wave solutions connecting u_+ and u_- spread with deterministic velocity $v \propto [V]$, where the potential jump is defined $[V] := V(u_-) - V(u_+)$. The finite critical radius means that nucleation events are localized, so that nucleation in one subsystem has negligible effect on behavior in neighboring subsystems. The traveling wave velocity, on the other hand, means that once nucleation has occurred, the spread of the new phase is deterministically driven, which is a great simplification.

3.1 Reduction to the Poisson Model in Large Systems

We propose partitioning the system into subsystems of length ℓ_ε where ℓ_ε is small enough that the exponential law (2.4) and the nucleation rate estimate (2.16) are valid approximations, but large enough that nucleation events on neighboring subsystems are asymptotically independent events. For validity of (2.4) and (2.16), the mean nucleation time should be large compared to the deterministic relaxation time of the system. This condition is expressed:

$$(\Lambda_\varepsilon^{\ell_\varepsilon})^{-1} (|\lambda_1^s| |\lambda_1^m|)^{1/2} \gg 1.$$

Because of (2.17), we therefore require $\ln \ell_\varepsilon \ll \varepsilon^{-1}$. For independence, on the other hand, the probability that there is no nucleation on $[-\ell_\varepsilon, \ell_\varepsilon]$ should be asymptotically equal to the product of the probability of no nucleation on $[-\ell_\varepsilon, 0]$ and the probability of no nucleation on $[0, \ell_\varepsilon]$; because of (2.4), we therefore require

$$\exp(-T \Lambda_\varepsilon^{2\ell_\varepsilon}) \approx (\exp(-T \Lambda_\varepsilon^{\ell_\varepsilon}))^2,$$

which in light of (2.16) and (2.17) translates into

$$\frac{\Delta E^{2\ell_\varepsilon}}{\varepsilon} - \frac{\Delta E^{\ell_\varepsilon}}{\varepsilon} = o(1)_{\varepsilon \rightarrow 0}. \tag{3.1}$$

Because the energy barrier converges exponentially with respect to ℓ_ε , (3.1) is satisfied if $\ell_\varepsilon \gg \ln \varepsilon^{-1}$. Hence, we choose a subsystem size satisfying

$$\ln \varepsilon^{-1} \ll \ell_\varepsilon, \quad \ln \ell_\varepsilon \ll \varepsilon^{-1}.$$

Using these heuristics, we define

$$L := L_\varepsilon / (\varepsilon^{1/4} \exp(\Delta E^\infty / 2\varepsilon)), \quad T := T_\varepsilon / (\varepsilon^{1/4} \exp(\Delta E^\infty / 2\varepsilon))$$

and estimate:

$$\begin{aligned} & \lim_{\varepsilon \rightarrow 0} \mathbb{P}(\text{no nucleation in } [0, L_\varepsilon] \times [0, T_\varepsilon]) \\ &= \lim_{\varepsilon \rightarrow 0} \mathbb{P}(\text{no nucleation in } [0, \ell_\varepsilon] \text{ for } t \leq T_\varepsilon)^{L_\varepsilon / \ell_\varepsilon} \\ &= \lim_{\varepsilon \rightarrow 0} \exp(-T_\varepsilon \Lambda_\varepsilon^{\ell_\varepsilon})^{L_\varepsilon / \ell_\varepsilon} \\ &= \lim_{\varepsilon \rightarrow 0} \exp\left(-\frac{L_\varepsilon T_\varepsilon \Lambda_\varepsilon^{\ell_\varepsilon}}{\ell_\varepsilon}\right) \\ &= \lim_{\varepsilon \rightarrow 0} \exp\left(-\frac{k L_\varepsilon T_\varepsilon}{\sqrt{\varepsilon} \exp(\Delta E^{\ell_\varepsilon} / \varepsilon)}\right) \\ &= \exp(-k L T) \end{aligned}$$

with

$$k = \frac{1}{(2\pi)^{3/2}} (|\lambda_1^s| |\lambda_1^m \lambda_2^m|)^{1/2} \prod_{j=3}^\infty (\lambda_j^m / \lambda_j^s)^{1/2} \|u'_s\|_{L^2(\mathbb{R})}.$$

Hence, under the space-time rescaling

$$x \rightarrow \frac{x}{\varepsilon^{1/4} \exp(\Delta E^\infty / 2\varepsilon)}, \quad t \rightarrow \frac{t}{\varepsilon^{1/4} \exp(\Delta E^\infty / 2\varepsilon)}, \tag{3.2}$$

we recover an exponential distribution of nucleation events

$$\mathbb{P}(\text{no nucleation on } [0, L] \times [0, T]) = \exp(-k L T). \tag{3.3}$$

The nucleation event looks like the generation of a single point of $u = u_+$ in the rescaled variables. Walls propagate from nucleation points with the deterministic velocity $v \propto [V]$. (By rescaling space and time equally, the slope is preserved.) The lower envelope of the graph divides the region of $u = u_-$ from the transformed region where $u = u_+$. ‘‘Virtual nucleation events’’ that fall above the lower envelope are rejected. (See Fig. 1 for an illustration.) This is the Poisson model, a simple version of a JMAK nucleation and growth model.

3.2 Dependence on System Size

The reduced model is useful to study the behavior of the SPDE in large systems. To compare the behavior on small, medium, and large systems, we choose as an observable the percent of transformed phase at time t :

$$R(t) := \frac{\mu(\{x; u(x, t) = u_+\})}{L},$$

where $\mu(\cdot)$ denotes Lebesgue measure. For simplicity, suppose that walls propagate with velocity $v = 1$.

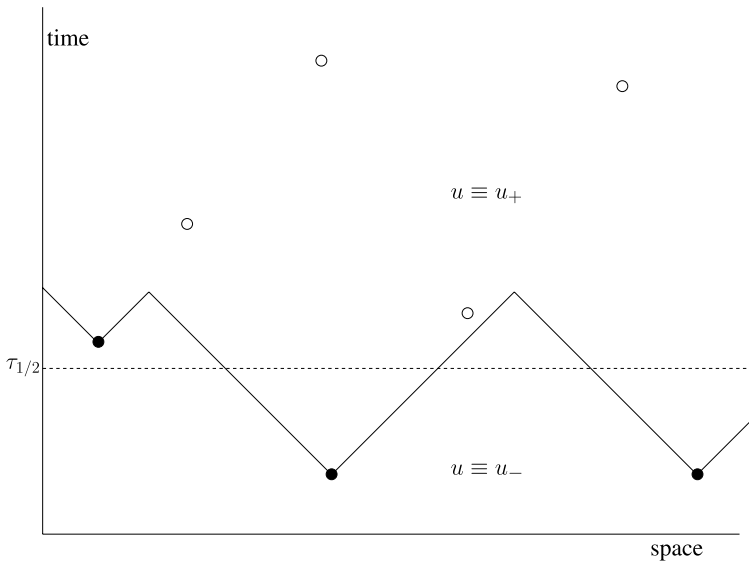


Fig. 1 The Poisson process with deterministic wall velocity. Nucleation events are points distributed in space-time with a rate coming from large deviation theory and prefactor estimates. Walls emerge from point nucleations with deterministically prescribed velocity. The lower envelope separates the untransformed region from the transformed region. (“Virtual nucleations” above the lower envelope are rejected)

Small Systems. For L order one in ε , the standard large deviation picture holds [15, 23, 38]. The timescale for phase transformation is indicated by the mean switching rate:

$$\Lambda_\varepsilon^L = C \exp(-\Delta E^L / \varepsilon).$$

On the associated timescale, the switching probability is Poisson,

$$\mathbb{P}(\text{no switch for } t \leq T) \approx \exp(-T \Lambda_\varepsilon^L).$$

The switching is “unpredictable,” in the sense that the mean and standard deviation are of the same order. A single nucleation event is expected and the walls cover the system in an order one time.

Medium Systems. The Poisson reduction suggests that for

$$L = O(\varepsilon^{1/4} \exp(\Delta E^\infty / 2\varepsilon)),$$

there is an order one probability of nucleation for the *dramatically increased rate*

$$\Lambda_\varepsilon^L = \varepsilon^{1/4} \exp(-\Delta E^\infty / 2\varepsilon).$$

(Dramatic because of the change by 1/2 in the exponential factor.) This is the “entropic effect” of the system size. The event $R(T) = \alpha$ depends on the distribution of nucleation events within the box $[0, L] \times [0, T]$.

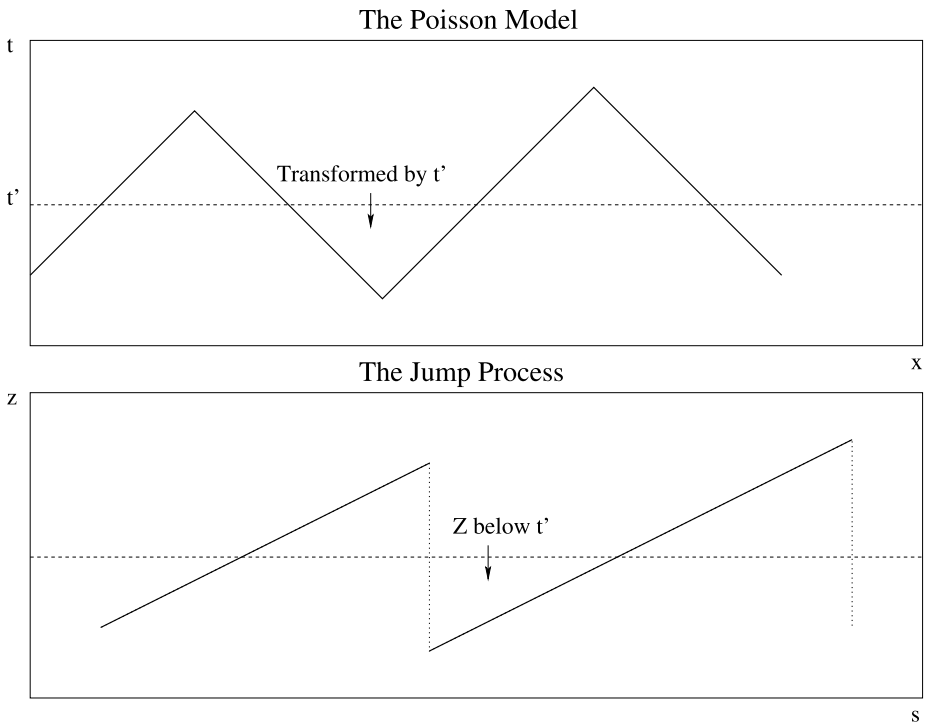


Fig. 2 The Poisson model and the jump process

Large Systems. For large systems

$$L \gg \varepsilon^{1/4} \exp(\Delta E^\infty / 2\varepsilon),$$

the Law of Large Numbers (LLN) leads to deterministic limiting behavior. The JMAK model [4, 11, 30, 31] allows one to quantify the effect. Recent work concerning LLN and Central Limit Theorem (CLT) results for JMAK models includes [13, 29, 41]. In the simple setting of the one-dimensional Poisson model with constant velocity and nucleation rate, it is easy to capture the LLN behavior. Consider a random variable $Z(s) : [0, S] \rightarrow \mathbb{R}^+$ such that Z propagates at a deterministic velocity $c > 0$, except for random times s' at which it jumps down to a point z , uniformly distributed on $[0, Z(s')]$. For $c = 1/2$, there is a one-to-one correspondence between the graph of this process and the lower envelope of the Poisson model, under the transformation $(x, t) = (s - z, z)$ (cf. Fig. 2). Furthermore, it is not hard to show that the normalized probability density $p_s(z, s)$ for $Z(s) = z$ has the stationary distribution,

$$p_s(z) = (z/\sqrt{c}) e^{-z^2/2\sqrt{c}}, \quad z > 0.$$

Consequently, we have

$$\lim_{S \rightarrow \infty} \frac{|\{s \in [0, S]; Z(s) > \alpha\}|}{S} = \int_\alpha^\infty p_s(z) dz.$$

Transformed into the language of the Poisson model, we obtain

$$\lim_{L \rightarrow \infty} R(t') = 1 - e^{-t'^2/\sqrt{2}} \text{ a.s.},$$

so that in particular, the time at which half the system is transformed is

$$\mathcal{T}_{1/2} = 2^{1/4} (\ln 2)^{1/2},$$

almost surely as $L \rightarrow \infty$.

4 Conclusion

We have proposed a methodology for studying rare events on large systems by breaking the domain into subsystems of intermediate scale on which “classical” results such as switching rate estimates and the exponential law can be applied. As an example, we have studied phase transformation for a scalar, one-dimensional, reaction-diffusion equation with white noise perturbation. We have drawn a connection between the large system limit of the SPDE and a simple JMAK nucleation and growth model. The formal reduction motivates the conjecture:

Conjecture 1 *There exists an ε -dependent rescaling of space and time and a random variable ξ mapping Ω to sets of points in the plane such that for every $\delta > 0, T > 0$, the rescaled solution of (1.2) (call it $\bar{u}(t, x, \omega)$) satisfies*

$$\mathbb{P} \left(\sup_{0 \leq t \leq T} \|\bar{u}(t, \cdot, \omega) - f(\xi(\omega))\|_{L^2} > \delta \right) \xrightarrow{\varepsilon \rightarrow 0} 0.$$

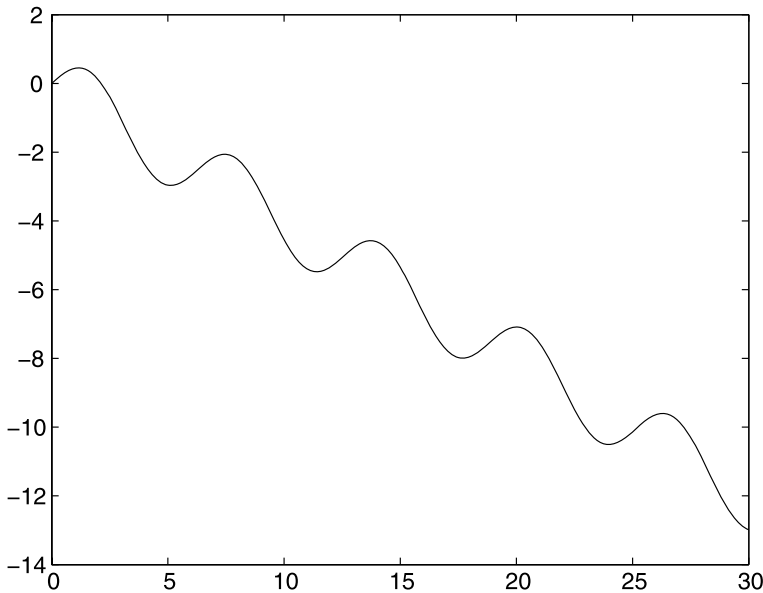


Fig. 3 A multi-well potential leads to a cascade of nucleations

Here, $f(\{a_i\}_{i=1}^{\infty})$ with $a_i \in \mathbb{R}^2$ is the function which is u_- (resp. u_+) below (resp. above) the lower envelope of the curve that is created by extending rays of slope ± 1 from each a_i .

One possible generalization of the SPDE reduction studied here is to the case of an asymmetric multi-well potential with infinitely many local minima, each with the same energy barrier between the minimum and the saddle to the right. (See Fig. 3.) In this case, there is a cascade of nucleations that generates “towers” whose heights grow without bound. The reduced model in this case is the PNG model studied in [42]. They connect the statistics of the height $H(x, t)$ with the longest increasing subsequence of a random permutation with Poisson distributed length, a quantity that is in turn connected to the largest eigenvalue of a random matrix [1, 5].

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