Noisy Classical Field Theories with Two Coupled Fields: Dependence of Escape Rates on Relative Field Stiffnesses

Lan Gong$^1$ and D. L. Stein$^{1,2}$

$^{1}$lan.gong@nyu.edu $^{2}$daniel.stein@nyu.edu

$^1$Department of Physics, New York University, New York, NY 10003

$^2$Courant Institute of Mathematical Sciences, New York University, New York, NY 10003

Abstract

Exit times for stochastic Ginzburg-Landau classical field theories with two or more coupled classical fields depend on the interval length on which the fields are defined, the potential in which the fields deterministically evolve, and the relative stiffness of the fields themselves. The latter is of particular importance in that physical applications will generally require different relative stiffnesses, but the effect of varying field stiffnesses has not heretofore been studied. In this paper, we provide a complete treatment of a model with two coupled fields, and explore the complete phase diagram of escape times as they depend on the various problem parameters. In addition to finding a transition in escape rates as the relative stiffness varies, we also observe a critical slowing down of the string method algorithm as criticality is approached.

1 Introduction

In a previous paper \cite{GS}, the authors introduced and solved a system of two coupled nonlinear stochastic partial differential equations. Such equations are useful for modelling noise-induced activation processes of spatially varying systems with multiple basins of attraction. Examples of such processes include micromagnetic domain reversal \cite{23}, pattern nucleation \cite{46}, transitions in hydrogen-bonded ferroelectrics \cite{7}, dislocation motion across Peierls barriers \cite{8}, and structural transitions in monovalent metallic nanowires \cite{910}. It is the last problem in particular that the model introduced in \cite{GS} was constructed to analyze.

The GS model provided a mathematical realization of a stochastic Ginzburg-Landau field theory consisting of two coupled classical fields, denoted $\phi_1(z)$ and $\phi_2(z)$, defined on a linear domain of finite extent $L$. The model displayed several
interesting features, including a type of “phase transition” in activation behavior as \( L \) varied. The transition was driven by a change in the saddle state, from a uniform configuration at small \( L \) to a spatially varying one (“instanton”) at larger \( L \). This transition has been noticed and analyzed for the case of a single field \cite{11,12}, but had not been seen in the rarely studied case of a system with two coupled fields. Perhaps more remarkably, the system admitted an exact solution for the instanton state; such exact solutions are rare in the case of nonlinear field theories with a single field, much less a nontrivial system of coupled fields.

The introduction of two fields was required to study transitions among different quantized conductance states in non-axisymmetric nanowires. The axisymmetric case had previously been treated theoretically in \cite{9,13}. However, detailed studies using linear stability analysis by Urban et al. \cite{14} indicated that roughly 1/4 of all such transitions involved either non-axisymmetric initial or final states, or else a least-action transition passing through a non-axisymmetric saddle. To describe such transitions, one field \((\phi_1(z))\) describes radial variations along the wire length and the other \((\phi_2(z))\) describes deviations from axisymmetry.

One restriction of the analysis in GS was that the respective bending coefficients \(\kappa_1\) and \(\kappa_2\) of the two fields were taken to be equal. However, this is generally not the case in real nanowires \cite{14}. Therefore, in order to apply the model to actual transitions, as well as to provide a complete picture of the activation behavior in such systems, we need to consider the case where \(\kappa_1 \neq \kappa_2\). In such cases analytical solutions cannot be found and we need to rely on numerical methods. The study of this more general problem is the subject of this paper.

2 The Model

Consider two coupled classical fields \(\phi_1(z), \phi_2(z)\) on the interval \([-L/2, L/2]\), subject to the energy functional

\[
\mathcal{H} = \int_{-L/2}^{L/2} \left( \frac{1}{2} \kappa_1 (\phi_1'(z))^2 + \frac{1}{2} \kappa_2 (\phi_2'(z))^2 + U(\phi_1, \phi_2) \right) dz .
\]
where

\[ U(\phi_1, \phi_2) = -\frac{\mu_1}{2} \phi_1^2 + \frac{1}{4} \phi_1^4 - \frac{\mu_2}{2} \phi_2^2 + \frac{1}{4} \phi_2^4 + \frac{1}{2} \phi_1^2 \phi_2^2 \]  

(2)

The bending coefficients \( \kappa_1, \kappa_2 \) can be related to the wire surface tension. The arbitrary positive constants \( \mu_1, \mu_2 \) are chosen such that \( \mu_1 \neq \mu_2 \), breaking rotational symmetry. (The case \( \mu_1 = \mu_2 \) has been investigated analytically by Tarlie et al. [15] in the context of phase slippage in conventional superconductors.)

If the system is subject to additive spatiotemporal white noise, then their time evolution is governed by the pair of stochastic partial differential equations:

\[
\dot{\phi}_1 = \kappa_1 \phi''_1 + \mu_1 \phi_1 - \phi_3^1 + \phi_2^1 \phi_1^2 + \sqrt{2\epsilon} \xi_1(z,t), \\
\dot{\phi}_2 = \kappa_2 \phi''_2 + \mu_2 \phi_2 - \phi_3^2 + \phi_2^1 \phi_2^2 + \sqrt{2\epsilon} \xi_2(z,t),
\]

(3)

where \( \xi_{1,2} \) are the spatiotemporal noise terms satisfying \( <\xi_i(z_1,t_1)\xi_j(z_2,t_2)> = \delta(z_1-z_2)\delta(t_1-t_2)\delta_{ij}, \ i, j = 1, 2 \). If the noise is due to thermal fluctuations, then by the fluctuation-dissipation theorem \( \epsilon = k_B T \).

The metastable and saddle states are time-independent solutions of the zero-noise equations:

\[
\kappa_1 \phi''_1 = -\mu_1 \phi_1 + \phi_3^1 + \phi_1^2 \phi_2^2 \\
\kappa_2 \phi''_2 = -\mu_2 \phi_2 + \phi_3^2 + \phi_2^1 \phi_1^2
\]

(4)

Without loss of generality, we choose \( \mu_1 > \mu_2 \). Then there are two metastable states: \( \phi_{1,s} = \pm \sqrt{\mu_1}, \phi_{2,s} = 0 \); two spatially uniform saddle states: \( \phi_{1,u} = 0, \phi_{2,u} = \pm \sqrt{\mu_2} \); and spatially nonuniform saddle states, or instantons, given by Eqs. (5) and (6).

\[
\phi_{1,m}^{\text{inst}}(z) = \pm \sqrt{m} \sqrt{2\mu_1 - \mu_2} - m(\mu_1 - \mu_2) \text{sn}(\sqrt{\mu_1 - \mu_2} z|m) \\
\phi_{2,m}^{\text{inst}}(z) = \pm \sqrt{m} \sqrt{2\mu_2 - \mu_1} - m(\mu_1 - \mu_2) \text{dn}(\sqrt{\mu_1 - \mu_2} z|m)
\]

(5)  (6)

where \( \text{sn}(.,|m) \) and \( \text{dn}(.,|m) \) are the Jacobi elliptic functions with parameter \( m \).

We found in GS that varying \( L \) triggers a transition between the uniform and instanton saddle states, resulting in a transition in the activation behavior, including anomalous behavior at the critical length. We will show below that the same effect occurs when the ratio \( \kappa_1/\kappa_2 \) is varied.
The transition rate in the low-noise ($\epsilon \to 0$) limit is given by the Kramers formula:

$$\Gamma \sim \Gamma_0 \exp(-\Delta E/\epsilon) \quad (7)$$

Here $\Delta E$ is the activation barrier, that is, the difference in energy between the saddle and the starting metastable states, while $\Gamma_0$ is the rate prefactor:

$$\Gamma_0 = \frac{1}{\pi} \sqrt{\frac{\det \Lambda_s}{\det \Lambda_u}} |\lambda_{u,1}|. \quad (8)$$

In the above equation $\Lambda_s$ is the linearized dynamical operator describing perturbations about the metastable state; similarly $\Lambda_u$ describes perturbations about the saddle. $\lambda_{u,1}$ is the single negative eigenvalue of $\Lambda_u$, corresponding to the direction along which the most probable transition path approaches the saddle state. The behavior of $\Gamma_0$ becomes anomalous at the critical point $L_c$, where fluctuations around the most probable path become large.

### 3 Calculation of the Minimum Energy Path

Computation of exit behavior requires knowledge of the transition path(s), in particular behavior near the local minimum and the saddle. In our model, both are found as solutions of two coupled nonlinear differential equations [1]. A powerful numerical technique constructed explicitly for this type of problem is the “string method” of E, Ren, and Vanden-Eijnden [16, 17]. The algorithm proceeds by evolving smooth curves, or strings, under the zero-noise dynamics. These strings connect the beginning and final locally stable states, and in between the two ends each string contains a series of intermediate states called ”images”. The method is constructed so that the string evolves towards the most probable transition path. The evolution proceeds until the condition for equilibrium is reached:

$$[\delta \mathcal{H}]^\perp = 0 \quad (9)$$

where $\mathcal{H}$ is given by [1] and $[\delta \mathcal{H}]^\perp$ is its component perpendicular to the string.

Once equilibrium is reached, the string images correspond to the configurations sampled by the system at different stages of the activation process. The image with highest energy is the one nearest the saddle state. In order to get an accurate result, the distribution of images needs to be sufficiently fine-grained. In our computation, we used 61 images (including the two ends of the string);
because of the symmetry of our energy functional, the image in the middle corresponds to the saddle.

When such symmetry is absent and the location of the saddle needs to be determined with high precision, one can use an alternative method to the brute force one of simply increasing the number of images along the string. This alternative requires first finding a rough approximation of the most probable transition path, again using the string method but with a small number of images, and then switching to a "climbing image" algorithm in which one picks up an image that is believed close to the saddle and then drive it towards the saddle. The climbing force is obtained from inverting the energy gradient along the direction of the unstable eigenvector of the saddle state. Details can be found in [16,17].

We have found an analogue to critical slowing down in the current context: near criticality convergence of the string method becomes increasingly slow. Expanding the energy functional around the saddle reveals that the lowest stable eigenvalue vanishes to second order, leading to a rapid increase in relaxation time. This phenomenon will be further investigated in the following sections.

4 Results

We now turn to the case $\kappa_1 \neq \kappa_2$. To begin, we fix $\kappa_2 = 1$ and vary $\kappa_1$. We consider the cases where $\kappa_1$ is both less than and greater than 1.

When $\kappa_1 = 1$, $L_c = \pi \sqrt{\mu_1 - \mu_2}$. Below $L_c$, the saddle is spatially uniform, and above $L_c$ it is spatially varying [1]. The situation becomes more complicated when $\kappa_1 \neq 1$. Fig. 1 summarizes our results when $\mu_1 = 3$, $\mu_2 = 2$ and $L > L_c = \pi$ (for notational convenience, we continue to use $L_c$ to denote the critical length when $\kappa_1 = \kappa_2 = 1$). We find that as $\kappa_1$ increases, the spatial variation of the instanton becomes increasingly suppressed (not surprising given its increasing energy cost), until the instanton finally collapses to the uniform state.

Conversely, when $L < L_c$, the instanton state is retrieved for $\kappa_1 < 1$ (cf. Fig. 2). In Fig. 3 we plot the energy of the saddle state against $\kappa_1$ for both $L = 0.25$ and $L = 4.51$. In these figures the curve to the left of the dashed line is the instanton branch, which increases monotonically until it reaches a constant value, the latter corresponding to the energy of the uniform saddle state.

We next investigated the question of whether the transition from uniform
saddle to instanton (or vice-versa) as $\kappa_1$ varies occurs as a continuous crossover or as an abrupt phase transition. If the latter, then we also need to determine the order of the transition.

Figs. 1 and 2 together suggest that there is indeed a phase transition as $\kappa_1$ varies for fixed $L$, and moreover that the transition is second-order (similarly to that induced by changing $L$ at fixed $\kappa_1$ [1]). Further evidence is provided by the divergence in the transition rate prefactor as shown in Fig. 4. The value of $\kappa_{1c}$ in Fig. 3 was determined as the value of $\kappa_1$ where the activation energies of the uniform and instanton saddles crossed. The value of $\kappa_{1c}$ determined in this way agrees with the value where the prefactor diverges to within a numerical error of $10^{-2}$.

We have studied a wide range of values of $L$, all of which lead to the same conclusion. Fig. 5 shows the divergence of $\Gamma_0$ at different $L$’s. This can be used to determine a relation between $\kappa_{1c}$ and $L_c$ in the following way. Away from criticality, the spectrum of the linearized dynamical operator $\Lambda$ about the saddle consists of a single negative eigenvalue, whose corresponding eigenvector determines the unstable direction, with all other eigenvalues positive. As criticality is approached, the smallest positive eigenvalue — call it $\lambda_{u,2}$ — approaches zero. This signals the mathematical divergence (on the “normal” lengthscale of $O(\epsilon^{1/2})$) of fluctuations about the saddle, and by (8) is seen to lead to divergence of the prefactor. (For a discussion of how to interpret this “divergence”, see [18].)

The eigenvalue spectrum about the uniform saddle can be analytically calculated [1]. In particular, $\lambda_{u,2} = \frac{\kappa^2}{L^2} - (\mu_1 - \mu_2)$. At fixed $L$, this switches from negative (unstable) to positive (stable) as $\kappa_1$ increases, as shown in Fig. 6. This change of sign corresponds to a transition from an instanton saddle to a uniform one as $\kappa_1$ varies.

Using this approach, the phase separation curve $L_c$ vs. $\kappa_{1c}$ can be derived analytically and the full phase diagram determined, as shown in Fig. 7. In this figure the solid line was analytically determined using the method just described and the dots represent transition values determined by numerics, as described earlier.
5 Discussion

We have solved the general two-field model of ¹ and ² for its full parameter space. We close with some remarks about the string method as applied to this problem.

A randomly placed string will relax towards the most probable transition path along the stable direction of the saddle. In Sec. ⁴ we defined the smallest positive eigenvalue (corresponding to the stable direction) of the linearized operator $\Lambda_u$. As a second-order phase transition is approached, $\lambda_{u,2}$ drops to $0^+$, so that the energy landscape curvature in the stable direction becomes very small. When the string arrives in its neighborhood, the restoring force exerted along its normal direction correspondingly becomes small leading to slow convergence. If one sits right at the critical point, the string will not arrive at the saddle.

The string method assumes that most of the probability flux from the reactant to the product state is carried by one (or more generally a few) paths through the saddle state, in each of which the probability flux is tightly confined to a narrow quasi - 1D region in state space. However, near criticality the path splays out in the direction normal to the longitudinal transition path. In this case one needs to consider transition “tubes”, inside which most of probability flux is concentrated. The equilibrium condition ³ corresponds to conditions away from criticality, where the transition tube is thin.

The equation for the path of max flux is derived in ¹⁹, where it is noted that the reaction flux intensity must be maximized along the thin transition tube (or the string, when using the string method). An alternative derivation can be found in ²⁰.

Acknowledgments. The authors are grateful to Weiqing Ren and Ning Xuan for helpful discussions. We are especially grateful to Gabriel Chaves for his help in programming the string method. This work was supported in part by NSF Grant PHY-0965015.

References


Figure 1: The evolution of the saddle state $\phi_{\text{saddle}}$ for $\mu_1 = 3$, $\mu_2 = 2$, and $L = 4.51$. $\kappa_1$ was increased from 1.95 to 2.20 with an increment of 0.01. The different colors here correspond to different $\kappa_1$’s. The arrows indicate the suppression of the instanton at $L > L_c = \frac{\pi}{\sqrt{\mu_1 - \mu_2}}$ as $\kappa_1$ increases.

Figure 2: The evolution of the saddle state $\phi_{\text{saddle}}$ for $\mu_1 = 3$, $\mu_2 = 2$, and $L = 0.25$. $\kappa_1$ was decreased from 1.0 to 0.5 with a decrement of -0.01. The different colors here correspond to different $\kappa_1$’s. The arrows indicate the retrieval of the instanton at $L < L_c = \frac{\pi}{\sqrt{\mu_1 - \mu_2}}$ as $\kappa_1$ decreases.
Figure 3: Energy of the saddle state as a function of $\kappa_1$. $\Delta E = E_{\text{saddle}} - E_{\text{metastable}}$. The dashed lines indicate that $\kappa_{1c} \approx 0.63$ for $L = 2.50$ and $\kappa_{1c} \approx 2.06$ for $L = 4.51$, where energies of the instanton and uniform saddles cross. Here $\mu_1 = 3$, and $\mu_2 = 2$.

Figure 4: $\Gamma_0$ diverges at $\kappa_1 = 2.06$. Here $\mu_1 = 3$, $\mu_2 = 2$, and $L = 4.51$. 
Figure 5: The divergence of $\Gamma_0$ at $L$ ranging from 2.6 to 5.0. Here $\mu_1 = 3$, $\mu_2 = 2$. The peaks are of different heights because the speeds of divergence are not necessarily the same for every $L$.

Figure 6: At $\mu_1 = 3$, $\mu_2 = 2$ and $L = 4.51$, the figure shows the smallest positive eigenvalue–$\lambda_{u_2}$–of the saddle state. The extended dashed line stands for that of the uniform saddle while below $\kappa_{1c}$. 
Figure 7: The phase diagram at $\mu_1 = 3$, $\mu_2 = 2$. The dots are $\kappa_{1c}$ at selected values of $L$ from numerics. The line corresponds to the situation when the smallest positive eigenvalue of uniform saddle is zero.