Droplet Nucleation and Domain Wall Motion in a Bounded Interval

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We study a spatially extended model of noise-induced magnetization reversal: a classical Ginzburg–Landau theory, restricted to a bounded interval and perturbed by weak spatiotemporal noise. We compute the activation barrier and Kramers prefactor. As the interval length increases, a transition between activation regimes occurs, at which the prefactor diverges. We relate this to transitions that occur in low-temperature quantum field theory.

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The effect of noise on spatially extended classical-mechanical systems has become a subject of intense investigation. Noise, by which is meant local fluctuations of thermal or other origin, may be spatiotemporal: it may vary randomly in space as well as time.

A typical problem is the determination of the extent to which spatiotemporal noise can induce transitions between the stable states of a system described by a nonlinear field equation, or induce such a system to escape from a metastable state. Langer and Büttiker and Landauer studied one-dimensional versions of this problem, in the limit of an infinite-size spatial region. Recently, finite size effects have become a subject of study and simulation. Micromagnetics is one application area. The thermally activated magnetization reversal of nanoscale magnets is described by coupled Landau–Lifschitz–Gilbert equations perturbed by spatiotemporal noise. An interesting question is how the effects of spatial extent cause magnetization reversal to differ from the better-understood ‘zero-dimensional’ case of a single-domain particle, with the noise taken to have no spatial dependence.

Another area where activation by spatiotemporal noise is important is the formation of spatially localized structures in electroconvection.

In this Letter, we quantify the effects of weak spatiotemporal noise on an overdamped bistable quartic (i.e., double well) classical Ginzburg–Landau field theory, in a one-dimensional region: the bounded interval \([0, L]\). This model is similar to that of Langer, and has much in common with the sine-Gordon model of Büttiker and Landauer. For sufficiently large \(L\), the model has two stable states, which are states of positive and negative magnetization. In the Kramers weak-noise limit, in which noise-activated magnetization reversals become exponentially rare, we compute the reversal rate \(\Gamma\). We also determine the ‘optimal trajectories’, in the model’s infinite-dimensional state space, for magnetization reversal. They are greatly affected by the choice of boundary conditions. If periodic boundary conditions are used, it is most likely that reversal will proceed via the nucleation of a droplet within a pair of Bloch walls; but for Dirichlet or Neumann boundary conditions, a single wall will form at \(x = 0\) or \(x = L\), and sweep across the interval. Faris and Jona-Lasinio worked out a mathematically rigorous ‘large deviation theory’ of the Dirichlet-case reversal.

Reversals fall off according to \(\Gamma \sim \Gamma_0 \exp(-\Delta E/\epsilon)\), where \(\epsilon\) is the noise strength, \(\Delta E\) is the activation barrier between the two states, and \(\Gamma_0\) is the Kramers prefactor. We show how to compute the prefactor in closed form, as a function of \(L\), for all three boundary conditions, and in the Dirichlet case, work it out in full. Langer computed it in the \(L \to \infty\) limit of the periodic case, so this is a significant advance. The prefactor contains a quotient of infinite-dimensional fluctuation determinants. Since the work of Coleman, the quantum field theory community has known how to compute such quotients as \(L \to \infty\). With the regularization technique of McKane and Tarlie, we can handle the \(L < \infty\) case, as well.

A feature of our prefactor computation is the calculation of the unstable eigenvalue of the model’s deterministic dynamics, at the transition state between its two stable states. The Kramers prefactor differs significantly from the analogous low-temperature quantum-mechanical tunneling prefactor, in that it involves this eigenvalue. Calculating it in the Dirichlet case is difficult. We express it in terms of a mid-band eigenvalue of the \(l = 2\) Lamé Hamiltonian. Using a dispersion relation developed for this Hamiltonian, we compute the eigenvalue, and hence the Dirichlet-case prefactor.

Our most striking discovery has to do with the phase structure of the weak-noise limit. In a sense that can be made precise, the \(\epsilon \to 0\) limit of the quartic Ginzburg–Landau theory has a second-order phase transition at \(L = 2\pi\) (Dirichlet, periodic cases) or \(L = \pi\) (Neumann case), in dimensionless units. At these critical values of the interval length, the Kramers prefactor diverges. This is due to the bifurcation of the transition state, as \(L\) increases through criticality. A zero-field ‘sphaleron’ configuration, which serves as transition state when \(L\) is small, bifurcates into a degenerate pair of ‘periodic instantons’. Similar bifurcations have been studied by the quantum field theory community. Until now, the importance of these bifurcations to classical activation by spatiotemporal noise has not been fully realized.

Model and Phenomenology.—In specifying the overdamped Ginzburg–Landau model, we follow Faris and Jona-Lasinio. On \([0, L]\), a classical field \(\phi = \phi(x,t)\) is evolved by the stochastic Ginzburg–Landau equation.
\[ \dot{\phi} = M\phi'' + \mu\phi - \lambda\phi^3 + \epsilon^{1/2}\xi(x,t), \]

where \( \xi(x,t) \) is unit-strength spatiotemporal white noise, satisfying \( \langle \xi(x_1, t_1)\xi(x_2, t_2) \rangle = \delta(x_1 - x_2)\delta(t_1 - t_2) \). We set \( M = \mu = \lambda = 1 \), or equivalently use dimensionless units, in which the length unit is the nominal coherence length \( \sqrt{M/\mu} \), the field strength unit is \( \sqrt{\mu/\lambda} \), etc.

In the absence of noise, the time-independent solutions of (1) include the sphaleron \( \phi = 0 \), and \( \phi = \pm 1 \); the latter are the magnetized states in the Neumann and periodic cases. In the Dirichlet case, \( \phi(x = 0) = \phi(x = L) = 0 \) is imposed, so the magnetized states necessarily differ. It is easy to check that if \( \epsilon = 0 \), the so-called periodic instanton \( \phi = \phi_{\text{inst},m}(x) \) is a time-independent solution of (1) for any \( m \) in the range \( 0 < m < 1 \). Here (cf. [7])

\[ \phi_{\text{inst},m}(x) \equiv \sqrt{\frac{2m}{m+1}} \sin(x/\sqrt{m+1} | m), \]

where \( \sin(\cdot | m) \) is the Jacobi elliptic function with parameter \( m \), which has quarter-period \( K(m) \) [8]. This quarter-period decreases to \( \pi/2 \) as \( m \to 0^+ \), in which limit \( \sin(\cdot | m) \) degenerates to \( \sin(\cdot) \), and it increases to infinity as \( m \to 1^- \). One would expect the Dirichlet-case stable magnetized states to be \( \pm\phi_{\text{inst},m,D} \), with \( m_D \) determined implicitly by the condition \( \phi(x = L) = 0 \), i.e., by the half-period condition \( 2\sqrt{m DN} + 1 K(m_D) = L \). However, this is so only if \( L > \pi \). If \( L \leq \pi \), there is no solution for \( m_D \) in the range \( 0 < m_D < 1 \), and the Dirichlet-case model is monostable with the zero-field configuration as its stable state, rather than bistable. Bistability disappears when \( L \to \pi^+ \) and \( m_D \to 0^+ \).

Noise-activated magnetization reversal, for weak noise, proceeds with high likelihood along an optimal trajectory in the model’s infinite-dimensional state space that goes ‘uphill’ from a magnetized state to an intermediate transition state. In a zero-dimensional approximation, this is the sphaleron. However, on physical grounds one expects a transition state to be an unstable field configuration with two droplets, i.e., with half the interval occupied by each magnetization value. Mathematically, this can arise as follows. In the Dirichlet case, the sphaleron undergoes a pitchfork bifurcation into the degenerate magnetized states \( \pm\phi_{\text{inst},m,D} \) when \( L \) is increased through \( \pi \). When \( L \) is increased through \( 2\pi \), it bifurcates again, into a degenerate pair of unstable states \( \pm\phi_{\text{inst},m,D} \). Unlike the magnetized states, these transition states are positive on half the interval and negative on the other. \( m_D \) is determined from \( L \) by the condition \( \phi(x = L) = 0 \), i.e., by the quarter-period condition \( 4\sqrt{m_D} + 1 K(m_D) = L \).

The same bifurcation occurs if periodic boundary conditions are used, but the new transition state is infinitely degenerate: it is \( \phi_{\text{inst},m,D} \) translated arbitrarily. It is easy to see that in the Neumann case, the bifurcation occurs at \( L = \pi \) rather than \( L = 2\pi \), with the Neumann parameter \( m_N \) determined by the half-period condition \( 2\sqrt{m_N} + 1 K(m_N) = L \). In fact, \( m_N = m_D \).

To satisfy Neumann boundary conditions, the field configurations \( \pm\phi_{\text{inst},m,D,N} \) must be shifted by \( L/2 \).

Figure 1 displays the magnetization and transition states for each boundary condition. As \( L \to \infty \), the Bloch walls between magnetization values increasingly acquire the standard hyperbolic tangent form, since \( \sin(\cdot | m) \) degenerates to \( \tanh(\cdot) \) as \( m \to 1^- \).

The zero-noise dynamics of this model are of the gradient form \( \phi = -\delta\mathcal{H}/\delta\phi \), with the energy functional

\[ \mathcal{H}[\phi] \equiv \int_0^L \left[ (\phi')^2/2 + \phi^4/4 - \phi^2/2 + 1/4 \right] dx. \]

The energy of each magnetization and transition state is readily computed from (3). The states \( \phi = \pm 1 \) have zero energy, and the sphaleron has energy \( L/4 \). The energy of each periodic instanton state \( \pm\phi_{\text{inst},m} \) turns out to be

\[ \mathcal{E}(m) = \frac{L}{12} \left[ \frac{8}{(m + 1)^2} \mathcal{K}(m) - (1 - m)(3m + 5) \right]. \]

where \( \mathcal{E}(m) \) is the second complete elliptic integral [10].

Figure 2 plots the activation barrier \( \Delta E \) as a function of \( L \), for each boundary condition. The second derivative of each \( \Delta E \) function is discontinuous at the value of \( L \) at which bifurcation occurs. As \( L \to \infty \), the value of \( \Delta E \) converges to the energy of a Bloch wall (Dirichlet, Neumann cases), or two Bloch walls (periodic case). It follows from (3) that the energy of a Bloch wall, of the \( m = 1^- \) limiting form \( \tanh(x/\sqrt{2}) \), is \( 2\sqrt{2}/3 \approx 0.943 \).

**Determinant Quotients.**—The formula for the Kramers prefactor \( \Gamma_0 \) of an overdamped multidimensional system driven by weak white noise is well known. Suppose the system has a stable state \( \varphi_s \) and a transition state \( \varphi_u \), with a single unstable direction. Let \( \Lambda_s \) and \( \Lambda_u \) denote the system’s linearized noiseless dynamics at \( \varphi_s \) and \( \varphi_u \), so that to leading order, the state \( \varphi = \varphi_s + \eta \) evolves by \( \dot{\eta} = -\Lambda_s\eta \), and \( \varphi = \varphi_u + \eta \) by \( \dot{\eta} = -\Lambda_u\eta \). Then [19]

![FIG. 1. Stable magnetized states (S) and transition states (U), for Dirichlet (D), Neumann (N), and periodic (P) boundary conditions, if \( L = 10 \). Each state may be multiplied by \(-1\), and UP may be shifted arbitrarily.](image)
yields the determinant quotient \( \Upsilon \), where

\[
\lambda_{\text{s},1} = \text{the smallest eigenvalue of } \mathbf{\Lambda}_{\text{s}}.
\]

If \( \lambda_{\text{s},1} \) denotes the smallest eigenvalue of \( \mathbf{\Lambda}_{\text{s}} \), the corresponding eigenvector \( \eta_{u,1} \) will be the direction along which the trajectory extends from the stable state.

Linearizing the noiseless version of (1) at a stationary state \( \dot{\phi}_0 \) (either a stable or a transition state) yields

\[
\dot{\eta} = -\dot{\Lambda}[\phi_0] \eta - \left[ -\frac{d^2}{dx^2} + (-1 + 3\phi_0^2) \right] \eta.
\]

So \( \Gamma_0 \) depends on the spectrum of the \( \dot{\Lambda} \) operators associated with the stable and transition states. In the Dirichlet case, the formal determinant quotient \( \Upsilon \) can be computed by the now standard technique of Coleman [8]. If \( L > 2\pi \), let \( \eta_{s,*} \) and \( \eta_{u,*} \) be the solutions on \([0, L]\) of the homogeneous equations \( \dot{\Lambda} [\phi_{\text{inst}, m, D}] \eta = 0 \) and \( \dot{\Lambda} [\phi_{\text{inst}, m, D}] \eta = 0 \) which satisfy the boundary conditions \( \eta(0) = 0 \) and \( \eta(0) = 1 \). Then, it turns out,

\[
\Upsilon_D = \frac{\eta_{s,*}(L)}{\eta_{u,*}(L)}.
\]

is the Dirichlet-case determinant quotient.

Solutions \( \eta_{s,*} \) and \( \eta_{u,*} \) satisfying these special boundary conditions may be constructed by a clever trick [8]: differentiating the periodic instanton \( \phi_{\text{inst}, m} \), with respect to \( m \), setting \( m \) to \( m_{s,D} \) and \( m_{u,D} \) respectively, and normalizing. This procedure uses the formula for the derivative of \( \text{sn}(\bullet \mid m) \) with respect to \( m \) [20]. The result is

\[
\eta_{c,*}(L) = \pm \frac{L}{m_{c,D}^2 - m_{c,D} + 1} \left[ \frac{m_{c,D} + 1}{1 - m_{c,D}} \frac{E(m_{c,D})}{K(m_{c,D})} - 1 \right],
\]

for both \( c = s \) and \( c = u \) (\( \pm \) is positive and negative respectively). Substituting \( \eta_{s,*}(L) \) and \( \eta_{u,*}(L) \) into [8] yields the determinant quotient \( \Upsilon_D \).

The unbifurcated regime, i.e., \( \pi < L < 2\pi \), must be handled a bit differently. Since the transition state is the sphaleron, and not the periodic instanton \( \phi_{\text{inst}, m, D} \), \( \eta_{u,*}(L) \) cannot be computed from the above formula. But it is trivial to check that \( \eta_{u,*}(L) \) simply equals \( \sin L \).

The Neumann case is treated similarly to the Dirichlet (we omit the details), but the case of periodic boundary conditions is very different, at least in the bifurcated regime \( L > 2\pi \). The periodic instanton transition state is infinitely rather than doubly degenerate, and at any transition state, the linearized dynamical operator \( \dot{\Lambda} \) has a soft ‘collective mode’, with a zero eigenvalue. Equation (8) must be modified, but the regularization technique of McKane and Tarlie [2] can be used to work out the periodic-case Kramers prefactor [20]. It acquires an \( e^{-1/2} / 2 \) factor. As a result, the periodic-case reversal rate becomes non-Arrhenius when \( L \) is increased through \( 2\pi \). A similar non-Arrhenius reversal rate falloff is displayed, in the limit of zero spatial extent, by the stochastic Landau–Lifschitz–Gilbert equation [8], due to its space of magnetization values having a continuous symmetry.

The Unstable Eigenvalue.—The stumbling block in the analytic computation of the Dirichlet-case Kramers prefactor is the calculation of \( \lambda_{u,1} \), the single negative (unstable) eigenvalue of the deterministic dynamics, linearized at the transition state. If \( \pi < L < 2\pi \) and the transition state is the sphaleron, \( \lambda_{u,1} = \pi^2 / L^2 - 1 \) is trivial to verify. But computing \( \lambda_{u,1} \) and the corresponding eigenfunction \( \eta_{u,1} \) when \( L > 2\pi \) is much harder. \( \eta_{u,1} \) is of considerable physical interest, since it describes the way in which the optimal trajectories approach the periodic instanton solutions \( \pm \phi_{\text{inst}, m, D} \), i.e., the way in which the moving Bloch wall slows to a halt at \( x = L / 2 \).

Here we sketch the calculation of \( \lambda_{u,1} \) and \( \eta_{u,1} \) from the eigenvalue equation \( \dot{\Lambda} \eta = \lambda \eta \); details will appear elsewhere [21]. Introducing \( z \equiv x \sqrt{\mu_{u,0} + 1} \), and for simplicity, writing \( m \) for \( m_{u,D} \), converts the equation to

\[
\left[ -\frac{d^2}{dz^2} + 6m \text{sn}^2(z \mid m) \right] \eta = \mathcal{E} \eta,
\]

where the ‘energy’ \( \mathcal{E} \) equals \( (m + 1)(\lambda_{u,1} + 1) \). The interval \( 0 \leq z \leq 4\mathbf{K}(m) \) corresponds to \([0, L]\). Equation (8) is the \( l = 2 \) Lamé equation [22,23] which is a Schrödinger equation with a periodic potential, whose lattice constant is \( 2\mathbf{K}(m) \). Its Bloch wave spectrum is known to consist of three energy bands [22], each extending over the wavenumber range \(-\pi / 2\mathbf{K}(m) \leq \kappa \leq \pi / 2\mathbf{K}(m) \).

According to Hermite’s solution of the Lamé equation [22], Eq. (8) has solutions of the form

\[
\eta(z) = \prod_{i=1}^{\infty} \left\{ \frac{H(z \pm \alpha_i \mid m)}{\Theta(z \mid m)} \exp(\mp Z(\alpha_i \mid m) z) \right\},
\]

where \( \mathbf{H}, \Theta, \) and \( Z \) are the Jacobi eta, theta, and zeta functions, and \( \alpha_1, \alpha_2 \) are certain complex constants determined by \( \mathcal{E} \). Clearly, the wavenumber \( k \) of the solution (8) equals \( \pm \text{Im} \sum_{i=1}^{\infty} Z(\alpha_i \mid m) \).
Everting this, we obtain an energy $E \mapsto \pm k$.

Stable eigenvalue

corresponding to $k = \pm \pi/4K(m)$, and hence the eigenvalue $\lambda_{u,1}$.

The difficulty lies in finding closed-form expressions for $\alpha_1, \alpha_2$ which will yield a solution $\eta = \eta_{u,1}(z)$ that satisfies Dirichlet boundary conditions on $0 \leq z \leq 4K(m)$. But $\eta_{u,1}$, being a ground state, should have no nodes, so it should extend to a periodic function with period $8K(m)$. That is, its wavenumber should be $\pm \pi/4K(m)$. One of us [13] has found expressions for $\alpha_1, \alpha_2$ in terms of $E$, which yield a dispersion relation $E \mapsto \pm k$. By inverting this, we obtain an energy $E$ corresponding to $k = \pm \pi/4K(m)$.

The divergence can be viewed as arising from the bifurcation of the optimal weak-noise reversal trajectory, rather than the bifurcation of the transition state on which it terminates. We previously found a similar prefactor divergence in a symmetric two-dimensional nonequilibrium model, whose optimal trajectory bifurcates but whose transition state does not [2], [16].

A natural question is whether the second-order phase transition is robust. In slightly more complicated classical field theories perturbed by spatiotemporal noise, such transitions may be first-order rather than second-order, with a discontinuous, rather than diverging, prefactor. Kuznetsov and Tinyakov [15] have studied stationary field configurations in a sixth-degree Ginzburg–Landau theory, with $\phi + a\phi^3 - (a + 1)\phi^5$ replacing the $\phi - \phi^3$ terms of ($\mathbf{6}$). The $\alpha = -1$ case is the theory we have treated. If $\alpha > -1$, the periodic instanton branch of the energy function crosses the sphaleron branch at a nonzero angle. This would give rise to a first-order transition. So, in the $(L, \alpha)$ plane, the second-order transition point $(2\pi, -1)$ must be the endpoint of a first-order transition curve.

To sum up, we have shown that taking spatial extent into account, in simple models of magnetization reversal induced by weak noise, may yield a rich structure of activation regimes separated by phase transitions. The choice of boundary conditions plays a major role. We expect more sophisticated models, and the phenomenon of field-induced reversal, will display similar structure.

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