Optimal Paths for Spatially Extended Metastable Systems Driven by Noise

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The least action principle is exploited as a simulation tool to find the optimal dynamic path for spatially extended systems driven by a small noise. Applications are presented for thermally activated switching of a spatially-extended bistable system as well as the switching dynamics of magnetic thin films. The issue of nucleation versus propagation is discussed and the scaling for the number of nucleation events as a function of the terminal time and other material parameters is computed.

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Thermal and other noises play a very important role in the behavior of many systems. No matter how small the noise is, it always has a non-trivial effect on long enough time intervals. Thermal noise has an especially important role for micro- or nano-devices since the energy barrier between metastable states may come close to \( k_B T \) in such systems and it may in fact limit the smallest size of such devices. One example is found in magnetic recording industry where the superparamagnetic limit, below which the data retention time becomes too short for commercial purposes, is now considered a serious limiting factor for the maximally achievable storage density. In order to better control such processes, it is necessary to first obtain a detailed quantitative understanding of the effect of the noises in such systems. For bistable systems that are often used in storage and memory applications, issues such as the mean switching time and the dynamics of the switching path have to be addressed. A major challenge is that most systems of interest are spatially extended and switching cannot be described using only a few degree of freedom. For instance, magnetization reversal in micron-sized magnetic films proceeds by nucleation and domain wall motion instead of coherent rotation. Predictions of reversal rates based stochastic coherent rotation models are off by orders of magnitude. In these cases, one has to deal with the added complexity of stochastic partial differential equations.

Traditionally the methods of choice for a quantitative understanding of the effect of noise have been the Monte Carlo method or direct simulation of the Langevin equation. For small level of noise, however, these methods become prohibitively expensive. While the maximal time step for Monte Carlo or Langevin simulations is still restricted by the deterministic part of the dynamics, the effect of the noise is significant only on time scales which are exponentially large in the inverse of noise amplitude. This time scale is the natural one for the noisy dynamics, and it is unaccessible by Monte Carlo or Langevin simulations. For instance, for the magnetic problem (of interest in magnetic recording), the timescale accessible to Monte Carlo or Langevin is on the order of nanoseconds, and the time scale of interest might be years.

In this paper we introduce a new numerical procedure to study spatially extended systems driven by a small noise. We are interested in the effect of rare events over long periods of time. Our method is based on the theory of large deviations which provides a least action principle for the most probable dynamic path. Even tough there has already been works using the least action principle for ordinary differential equations, extending this in the context of spatially extended systems present non-trivial numerical difficulties. In the examples we consider, namely thermally activated switching in a system with a bistable potential modeled by the Ginzburg-Landau equations in one and two dimensions and sub-micron-sized magnetic thin films, the numerical computations are non-trivial because switching proceeds by nucleation and domain wall motion which are both very localized in space and time, and require using very fine grids. Also, the diffusion terms present in these equations lead to very bad condition numbers, which results in a loss of accuracy as well as an increase of the numbers of iterations necessary for convergence. We introduce an efficient numerical method to overcome these problems which incorporates amongst other techniques the use of suitable preconditioners, efficient minimization techniques such as the Quasi-Newton method, etc.

Let us begin by considering the simplest continuum model describing the spatio-temporal states of a bistable system, namely the Ginzburg-Landau equation

\begin{equation}
\frac{\partial u}{\partial t} = \delta u_{xx} - \delta^{-1}V'(u),
\end{equation}

on the interval \([0, 1]\) with the boundary conditions \( u(0) = u(1) = 0 \). We take \( V \) to be a standard double-well potential, \( V(u) = \frac{1}{4}(1 - u^2)^2 \). \( \delta \) is expressed in appropriate dimensionless variables in which \( \delta \) is a small parameter which indicates that the reaction term, \( \delta^{-1}V'(u) \), is fast while the diffusion is slow. \( \delta \) can be considered as the gradient flow associated with the energy

\begin{equation}
E[u] = \frac{1}{2} \int_0^1 \left( \delta u_x^2 + 2\delta^{-1}V(u) \right) dx.
\end{equation}
The dynamics in (1) has two stable equilibrium states, $u_+$ and $u_-$, which minimize the energy (2). When $\delta$ is small, $u_\pm(x) = \pm 1$ except at a thin boundary layer of width $\delta$ at $x = 0, 1$ (see Fig. 1).

Now let us add to (2) a small noise term modeling thermal effects:

$$u_t = \delta u_{xx} - \delta^{-1}V'(u) + \sqrt{\varepsilon} \eta,$$

where $\varepsilon$ is proportional to the temperature of the system and $\eta$ is space-time Gaussian white noise with covariance

$$\langle \eta(x, t) \eta(y, s) \rangle = \delta(x - y) \delta(t - s).$$

The presence of the noise in (3) destroys the long-time stability of the equilibria $u_\pm$. For instance, if the initial state is $u_+$, there is a finite probability that the system switches to $u_-$ in any time interval $[0, T]$. To quantify the probability of such a switching or, in fact, any other event, one can introduce an action functional, $S_T[u]$, such that for small $\varepsilon$, the probability that the solution $u$ of (2) is close to a given path $\varphi$ on $[0, T]$ can be estimated by

$$\text{Prob}\{u \approx \varphi\} \sim \exp(-\varepsilon^{-1}S_T[\varphi]).$$

The action functional corresponding to (3) is given explicitly by

$$S_T[u] = \int_0^T \int_0^1 \left(u_t - \delta u_{xx} + \delta^{-1}V'(u)\right)^2 dx dt.$$

The large deviation principle in (6) allows us to estimate the probability of various events associated with (3) by constrained minimization of the action functional (6).

For instance, the probability $P_T$ that the system switches from $u_+$ to $u_-$ before time $T$ satisfies

$$\lim_{\varepsilon \to 0} \varepsilon \ln P_T = -\min_u \{S_{0, T}[u]\},$$

where the minimization in (7) is constrained by the boundary conditions

$$u|_{x=0} = u|_{x=1} = 0, \quad u|_{t=0} = u_+, \quad u|_{t=T} = u_-.$$

Furthermore assume that the system switches before time $T$. Then the minimizer of (7) gives the optimal switching path between $u_+$ and $u_-$ during the time interval $[0, T]$, in the sense that the probability that the system switches by another path is exponentially smaller in $\varepsilon$.

To find the optimal path, we numerically minimize the action functional, subject to the boundary condition in (8). We put down a numerical grid on the space-time domain $(0, 1) \times [0, T]$. The action functional (6) is discretized using finite difference formulas. Numerical optimization is implemented using a Quasi-Newton method, the BFGS method (8). In order to speed up convergence, we used the operator obtained from minimizing the linear part of (6), $\int_0^T \int_0^1 (u_t - \delta u_{xx})^2 dx dt$, as the preconditioner. Similar procedures were used for the other examples below and numerical details are provided in (9).

Figure 2 shows the sequence of profiles of $u$ at different times in $[0, T]$ for various values of $T$ at a fixed $\delta$. The switching proceeds by nucleation followed by propagation of domain walls. For large $T$, the switching proceeds by propagating a domain wall from one boundary to the other. As $T$ becomes smaller, however, the number of nucleation events increase. Such switching scenario with multi-nucleations are relevant at finite temperature (10). In Figure 2 where we display the values the action for the various local minimizers, plotted against $T$. FIG. 2 shows the space-time plot of $(u_t - \delta u_{xx} + \delta^{-1}V'(u))^2$ during a switching event. This
corresponds to the minimal (squared) noise necessary to make a switching.

These results can be understood as follows. Consider the critical points of the energy (3), i.e. the solutions of $0 = \delta u_{xx} - \delta^{-1} V'(u)$ with $u|_{x=0} = u|_{x=1} = 0$. Besides $u_+$ and $u_-$, corresponding to the minimizers of the energy, there are also saddle point configurations, denoted by $u_S$, with an increasing number of domain walls. For each saddle point, there is a path joining $u_+$ to $u_-$ through that saddle point. Our result shows that, for large $T$, the switching path crosses the saddle point configuration with minimum energy, i.e the configuration with a single domain wall (see (a) in Figure 3). As $T$ is decreased, one might naively think that the switching will occur via the same path followed at a faster rate. This intuition is wrong. For smaller $T$, the optimal switching path crosses a saddle point configuration with increasing energy, i.e. more nucleations and therefore more domain walls, giving rise to the cascade of nucleation events seen in Figure 3. The reason is simply that both nucleation and domain wall motion are noise induced. As $T$ decreases, at fixed number of nucleations the speed of propagation of the domain wall must increase in order to achieve complete switching during the allowed time $T$. This is energy consuming and, at certain critical values of $T$ it becomes more favorable to make an additional nucleation.

The same type of cascade in the number of nucleations is also observed if $T$ is kept fixed but $\delta$ is decreased, because the cost of domain-wall motion increases as $\delta$ decreases, whereas the cost of a nucleation stays the same. In fact, a simple scaling argument gives $n_\star = C(\delta T)^{-1/2}$, for small $\delta$ and $T$, where $n_\star$ is the number of nucleations in the optimal switching path, and $C$ is a numerical constant. Furthermore, one has $\lim_{\varepsilon \to 0} \varepsilon \ln P_T = -C'(\delta T)^{-1/2}$, which gives the envelop of the curves in Fig. 2. The detailed analysis of the cascade process of nucleations will be presented elsewhere.

As an example in two dimensions, we minimize

$$S_T[u] = \int_0^T \int_{\Omega} (u_t - \delta \Delta u + \delta^{-1} V'(u))^2 \, dx \, dt,$$

where $\Omega$ is the unit square, $\Omega = [0,1] \times [0,1]$. We will present results with two different boundary conditions: (i) $u = 1$ at $x = 0$ and $x = 1$, $u = -1$ at $y = 0$ and $y = 1$, and (ii) $u = 0$ on the edge of the square. In both cases there are two global minimizers of the energy. One minimizer, $u_+$, is close to $u = 1$ except for the boundary layers at $y = 0$ and $y = 1$ (case (i)) or at the edge of square (case (ii)). The other minimizer, $u_-$, is close to $u = -1$ except for the boundary layers at $x = 0$ and $x = 1$ (case (i)) or at the edge of square(case (ii)). In the absence of noise, both minimizers are stable equilibrium states.

In Figure 4, we show the time sequences of the switching process for different values of $\delta$ at fixed $T$. The overall trend is consistent with what was found in the previous example, namely there are more and more nucleation events as $\delta, T \to 0$.

Finally let us consider thermally activated switching of a magnetic thin film, modeled by the Landau-Lifshitz-Gilbert equation, which after suitable nondimensionalization, reads

$$m_t = f(m) := -m \times h_{\text{eff}} - \alpha m \times (m \times h_{\text{eff}}).$$

Here $m$ is the magnetization distribution (3d vector) which satisfies $|m| = 1$, $h_{\text{eff}}$ is the effective local field, given in terms of the free energy by $h_{\text{eff}} = -\delta E[m] / \delta m$. 

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**FIG. 3:** Space-time value of $(u_t - \delta \Delta u + \delta^{-1} V'(u))^2$ for the minimizer (f) in Fig. 2. This can be interpreted as the minimal noise necessary for switching: the noise induces the nucleations then propagates the domain walls. The peaks correspond to nucleations.

**FIG. 4:** Snapshots of profiles of the minimizer $u$ during a switching from $u_+$ (top figure in one column) to $u_-$ (bottom figure in one column) at five equally spaced times on $[0, T]$ for $T = 1$ and different $\delta$ and different boundary conditions: (a)–(c) correspond to case (i), (d) to case (ii). In (a) $\delta = 0.04$; (b) $\delta = 0.03$; (c) $\delta = 0.01$; (d) $\delta = 0.01$. The gray-scale is from white for $u = -1$ to black for $u = +1$. 

to permalloy, and consider a thin square domain of size
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where
\[ E[m] = \int_{\Omega} |\nabla m|^2 d^3x + \int_{\Omega} \phi(m) d^3x + \int_{\mathbb{R}^3} |\nabla u|^2 d^3x. \]

Here the three terms represent respectively energies due to exchange, anisotropy, and stray field. \( \Omega \) is the region occupied by the magnetic thin film. The potential \( u \), defined everywhere in space, solves \( \text{div} (-\nabla u + m) = 0 \), where \( m \) is extended as 0 outside the sample.

The first term at the right hand side of (10) describes precession of \( m \) around \( h_{\text{eff}} \); the second term, which can be written as \(-\alpha m \times (m \times h_{\text{eff}})\), is a damping term whose strength is measured by the parameter \( \alpha \). We choose physical parameters corresponding to permalloy, and consider a thin square domain of size \( 200nm \times 200nm \times 10nm \).

The dynamics in (10) has equilibrium states corresponding to the minima of the magnetic energy, \( E[m] \). Thermal noise effects can be represented by modifying \( h_{\text{eff}} \) as \( h_{\text{eff}} \sim \sqrt{\varepsilon} \eta \), where \( \eta \) is a vector white-noise, and will eventually switch the system from one minimum to any other one. In Fig. 5 (m1) and (m4) show two minima where the magnetization points mostly to the right (white color) or to the left (black color), respectively. For small noise, the optimal path for a switching from (m1) to (m4) during the time interval \([0, T]\) is obtained by minimizing the action functional corresponding to (10):

\[ S_T[m] = \int_0^T \int_{\Omega} |m_t - f(m)|^2 d^3x d\tau. \]  

The global minimizer of (11) on a long time interval, \( T = 450 \), is presented in Fig. 6. Looking at the energy \( E[m] \) during the switching one sees that two intermediate minima, (m2) and (m3), and three saddle configurations, (s1), (s2), and (s3), are crossed during the switching. The first step of the switching from (m1) to (m2) through (s1) rotates the interior magnetization by 90°. The second step from (m2) to (m3) through (s2), which is the most expensive step, switches magnetization at the top and bottom end domains. Finally, the third step from (m3) to (m4) through (s3) is similar to the first one.

In conclusion, we have shown that the least action principle can be turned into an efficient numerical procedure for finding the optimal dynamic path in spatially-extended systems driven by small noise, and we have presented applications to bistable systems modeled by the Ginzburg-Landau equation and the magnetic thin films. Our numerical method circumvents the difficulty of having to compute too many time steps in order to observe the relevant events. It is general and can be applied to a variety of problems in physics, chemistry as well as biology.

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