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CONVERGENCE ANALYSIS OF A FINITE ELEMENT APPROXIMATION OF MINIMUM ACTION METHODS*

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Abstract. In this work, we address the convergence of a finite element approximation of the minimizer of the Freidlin–Wentzell (F-W) action functional for nongradient dynamical systems perturbed by small noise. The F-W theory of large deviations is a rigorous mathematical tool to study small-noise-induced transitions in a dynamical system. The central task in the application of F-W theory of large deviations is to seek the minimizer and minimum of the F-W action functional. We discretize the F-W action functional using linear finite elements and establish the convergence of the approximation through Γ-convergence.

Key words. large deviation principle, minimum action method, convergence analysis, nongradient system, phase transition

AMS subject classifications. 65M60, 65P40, 65K10

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1. Introduction.

We consider a general dynamical system perturbed by small noise

$$dX = b(X)\,dt + \sqrt{\varepsilon}\,dW(t), \tag{1.1}$$

where ε is a small positive number and $W(t)$ is a standard Wiener process in $\mathbb{R}^n$. The long-term behavior of the perturbed system is characterized by the small-noise-induced transitions between the equilibriums of the unperturbed system

$$\frac{dx}{dt} = b(x), \quad x \in \mathbb{R}^n. \tag{1.2}$$

These transitions rarely occur but have a major impact. This model can describe many critical phenomena in physical, chemical, and biological systems, such as nonequilibrium interface growth [10, 18], regime change in climate [29], switching in biophysical networks [28], and hydrodynamic instability [21, 25, 24].

The Freidlin–Wentzell (F-W) theory of large deviations provides a rigorous mathematical framework to understand the small-noise-induced transitions in general dynamical systems, where the key object is the F-W action functional, and the critical quantities include the minimizer and minimum of the F-W action functional [11]. Starting from [6], the large deviation principle given by the F-W theory has been approximated numerically, especially for nongradient systems, and the numerical methods are, in general, called minimum action methods (MAMs). More specifically, the

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following optimization problems need to be addressed:

$$\text{Problem I:}\quad S_T(\phi^*) = \inf_{\substack{\phi(0)=x_1,\\ \phi(T)=x_2}} S_T(\phi) \tag{1.3}$$

and

$$\text{Problem II:}\quad S_{T^*}(\phi^*) = \inf_{T\in\mathbb{R}^+} \inf_{\substack{\phi(0)=x_1,\\ \phi(T)=x_2}} S_T(\phi), \tag{1.4}$$

where

$$S_T(\phi) = \frac{1}{2}\int_0^T |\phi' - b(\phi)|^2\, dt \tag{1.5}$$

is called the action functional. Here $\phi(t)$ is a path connecting x_1 and x_2 in the phase space on the time interval $[0, T]$. The minima and minimizers of Problems I and II characterize the difficulty of the small-noise-induced transition from x_1 to the vicinity of x_2; see (2.1) and (2.3). In Problem I, the transition is restricted to a certain time scale T, which is relaxed in Problem II. Let $\phi^*(t)$ be the minimizer of either Problem I or Problem II, which is also called the minimal action path (MAP) or the instanton in physical literature related to the path integral. For Problem II, we have an optimal integration time T^* which can be either finite or infinite depending on the states x_1 and x_2.

We will focus on the MAM for nongradient systems [7, 27, 30]. For gradient systems, the MAP is consistent with the minimum energy path, and the counterpart version of the MAM includes the string method [6, 8], the nudged elastic band method [15], etc., which takes advantage of the property that the MAP is parallel to the drift term of the stochastic differential equation. For nongradient systems, this property does not hold, and a direct optimization of the F-W action functional needs to be considered. The main numerical difficulty comes from the separation of slow dynamics around critical points from fast dynamics elsewhere. More specifically, the MAP will be mainly captured by the fast dynamics subject to a finite time, but it will take infinite time to pass a critical point. To overcome this difficulty, there exist two basic techniques: (1) nonuniform temporal discretization and (2) reformulation of the action functional with respect to arc length. Two typical techniques to achieve nonuniform temporal discretization include the moving mesh technique and the adaptive finite element method. The moving mesh technique starts from a uniform finite mesh and redistributes the grid points iteratively such that more grids are assigned into the region of fast dynamics and fewer grids into the region of slow dynamics. This technique is used by the adaptive minimum action method (aMAM) [31, 20, 23, 19]. The adaptive finite element method starts from a coarse mesh and has an inclination to refine the mesh located in the region of fast dynamics [22, 26]. The main difference between these two techniques from an efficiency point of view is that the moving mesh technique needs a projection from fine mesh to fine mesh, i.e., global reparameterization, while the adaptive finite element method only needs local projection in the elements that have been refined. To eliminate the scale separation from dynamics, one can consider parameterization of the curves geometrically, i.e., a change of variable from time to arc length, which is used in the geometric minimum action method (gMAM) [14, 12, 13]. The change of variable induces two difficulties. One is related to accuracy, and the other one is related to efficiency. The mapping from time to arc length is nonlinear, and the Jacobian of the transform between time and arc length variables is singular around critical points since an infinite time domain has been mapped to a finite arc length. Unknown critical points along the MAP may deteriorate the approximation accuracy unless they can be identified accurately. To use arc length for parameterization, we have that the velocity is a constant, which means that in each iteration step a global reparameterization is needed to maintain this constraint.

Both aMAM and gMAM target the case that $T^* = \infty$. In aMAM, a finite but large T is used, while in gMAM, the infinite T^* is mapped to a finite arc length. Thus, aMAM is not able to deal with Problem II subject to a finite T^* since a fixed T is required, while gMAM is not able to deal with Problem I since T has been removed. To deal with both Problems I and II in a more consistent way, we have developed a MAM with optimal linear time scaling (temporal minimum action method, or tMAM) coupled with adaptive finite element discretization [22, 26]. The method is based on two observations: (1) for any given transition path, there exists a unique T to minimize the action functional subject to a linear scaling of time, and (2) for transition paths defined on a finite element approximation space, the optimal integration time T^* is always finite but increases as the approximation space is refined. The first observation removes the parameter T in Problem II, and the second observation guarantees that the discrete problem of Problem II is well-posed after T is removed. Problem I becomes a special case of our reformulation of Problem II. In this way, tMAM is able to deal with both Problems I and II.

Although many techniques have been developed from the algorithm point of view, few numerical analyses have been done for the MAM. In this paper, we want to partially fill this gap. We consider a general stochastic ordinary differential equation (ODE) system (1.1). The discrete action functional $S_{T,h}$ will be given by linear finite elements for simplicity, where h indicates the element size. Due to the general assumption for $b(x)$, we will focus on the convergence of the minimizers of $S_{T,h}$ as $h \to 0$ and provide only an a priori error estimate for the approximate solution when $b(x)$ is a linear symmetric positive definite (SPD) system. For Problem I, the convergence of the minimizer ϕ_h^* to ϕ^* is established by the Γ-convergence [1, 2, 4] of the discretized action functional. For Problem II, we employ and analyze the strategy developed in [22] to deal with the optimization with respect to T. More specifically, we reformulate the problem from $[0, T]$ to $[0, 1]$ by a linear time scaling $s = t/T$ and replace the integration time T with a functional $\hat{T}(\bar{\phi})$ with $\bar{\phi}(s) = \phi(t/\hat{T})$, where $\hat{T}(\bar{\phi})$ is the optimal integration time for a given transition path $\bar{\phi}$. When T^* is finite, the convergence of the minimizer $\bar{\phi}_h^*$ to $\bar{\phi}^*(s) = \phi^*(t/T^*)$ can be established by the Γ-convergence of the discretized action functional. When $T^* = \infty$, the linear mapping from t to s does not hold. We demonstrate that the sequence $\{\bar{\phi}_h^*\}$ still provides a minimizing sequence as $h \to 0$ and establish the convergence using the results from gMAM. Due to the nonlinearity of $b(x)$, the Euler–Lagrange (E-L) equation associated with the action functional is, in general, a nonlinear elliptic problem for Problem I. For Problem II subject to an optimal linear time scaling, the E-L equation retains the same form as Problem I with the parameter T being replaced by a functional $\hat{T}(\bar{\phi})$, which becomes a nonlocal and nonlinear elliptic equation. When $b(x)$ is a linear SPD system, we are able to establish the a priori error estimate for $\bar{\phi}_h^*$, where the E-L equation is a nonlocal and nonlinear elliptic problem of Kirchhoff type.

The remainder of this paper is organized as follows. In section 2, we describe the problem setting. A reformulation of the F-W action functional is given in section 3 to deal with the optimization with respect to T in Problem II. We establish the convergence of finite element approximation in section 4 for general stochastic ODE systems. In section 5, we apply our method to a linear stochastic ODE system and provide an a priori error estimate of the approximation solution. Numerical illustrations are given in section 6, followed by a summary section.

2. Problem description. We consider the small-noise-perturbed dynamical system (1.1). Let x_1 and x_2 be two arbitrary points in the phase space. The F-W theory of large deviations provides asymptotic results to estimate the transition probability from x_1 to the vicinity of x_2 when $\varepsilon \to 0$. If we restrict the transition to a certain time interval $[0, T]$, we have

$$\lim_{\delta \downarrow 0} \lim_{\varepsilon \downarrow 0} -\varepsilon \log \Pr(\tau_\delta \leq T) = \inf_{\substack{\phi(0)=x_1,\\ \phi(T)=x_2}} S_T(\phi), \tag{2.1}$$

where τ_δ is the first entrance time of the δ-neighborhood of x_2 for the random process $X(t)$ starting from x_1. The path variable ϕ connecting x_0 and x_1, over which the action functional is minimized, is called a *transition path.* If the time scale is not specified, the transition probability can be described with respect to the quasi-potential from x_1 to x_2:

$$V(x_1, x_2) := \inf_{T \in \mathbb{R}^+} \inf_{\substack{\phi(0)=x_1,\\ \phi(T)=x_2}} S_T(\phi). \tag{2.2}$$

The probability meaning of $V(x_1, x_2)$ is

$$V(x_1, x_2) = \inf_{T \in \mathbb{R}^+} \lim_{\delta \downarrow 0} \lim_{\varepsilon \downarrow 0} -\varepsilon \log \Pr(\tau_\delta \leq T). \tag{2.3}$$

In general we refer to the asymptotic results given in (2.1) and (2.3) as the large deviation principle (LDP). We use ϕ^* to indicate the transition path that minimizes the action functional in (2.1) or (2.3), which is also called the minimal action path (MAP) [7]. The MAP ϕ^* is the most probable transition path from x_1 to x_2. For the quasi-potential, we let T^* indicate the optimal integration time, which can be either finite or infinite depending on x_1 and x_2. The importance of LDP is that it simplifies the computation of transition probability, which is a path integral in a function space, to seeking the minimizers ϕ^* or (T^*, ϕ^*). From the application point of view, one central task of the F-W theory of large deviations is to solve Problems I and II, defined in (1.3) and (1.4), respectively. For Problem II, we need to optimize the action functional with respect to the integration time T. We will present a reformulation of S_T in section 3 to deal with this case.

To analyze the convergence properties of numerical approximations for Problems I and II, we need some assumptions on $b(x)$.

ASSUMPTION 2.1.

(1) *$b(x)$ is Lipschitz continuous in a big ball; i.e., there exist constants $K > 0$ and $R_1 > 0$, such that*

$$|b(x) - b(y)| \leq K|x - y| \quad \forall\ x, y \in B_{R_1}(0), \tag{2.4}$$

where $|\cdot|$ denotes the ℓ_2 norm of a vector in $\mathbb{R}^n$.

(2) *There exist positive numbers β, R_2, such that*

$$\langle b(x), x \rangle \leq -\beta |x|^2 \quad \forall\ |x| \geq R_2, \tag{2.5}$$

where $R_2^2 \le R_1^2 - \frac{S^*}{\beta}$ *and*

$$S^* = \max_{x,y\in B_{R_2}(0)} \frac{1}{2}\int_0^1 \big|y - x - b\big(x + (y-x)t\big)\big|^2\, dt.$$

(3) *The solution points of* $b(x) = 0$ *are isolated.*

Lemma 2.2. *Let assumption* (2.5) *hold. If both the starting and ending points of a MAP* $\phi(t)$ *are inside* $B_{R_2}(0)$, *then* $\phi(t)$ *is located within* $B_{R_1}(0)$ *for any* t.

Proof. Suppose that $\phi(t)$ is a MAP outside of $B_{R_2}(0)$ but connecting two points x and y on the surface of $B_{R_2}(0)$. Let $w(t) = \phi' - b(\phi)$. We have

$$\phi' = b(\phi) + w. \tag{2.6}$$

Taking the inner product on both sides of the above equation with 2ϕ, we get

$$\frac{d|\phi|^2}{dt} = 2\langle b(\phi), \phi\rangle + 2\langle w, \phi\rangle. \tag{2.7}$$

Then by using Cauchy's inequality with β, and assumption (2.5), we get

$$\frac{d|\phi|^2}{dt} \le -2\beta|\phi|^2 + \frac{1}{2\beta}|w|^2 + 2\beta|\phi|^2 = \frac{1}{2\beta}|w|^2. \tag{2.8}$$

Taking integration, and using the definition of minimum action, we obtain a bound for any t along the MAP:

$$|\phi|^2 \le |x|^2 + \int_0^t \frac{1}{2\beta}|w|^2\, dt \le R_2^2 + \frac{1}{\beta}S_{T^*}(\phi) \le R_2^2 + \frac{1}{\beta}S^* \le R_1^2, \tag{2.9}$$

which means that the whole MAP is located within $B_{R_1}(0)$. ∎

Remark 2.3. The assumptions (2.4) and (2.5) allow most of the physically relevant smooth nonlinear dynamics. It is seen from Lemma 2.2 that the second assumption (2.5) is used to confine all MAPs of interest inside $B_{R_1}(0)$. For simplicity and without loss of generality, we will assume from now on that the Lipschitz continuity of $b(x)$ is global, namely, $R_1 = \infty$. For the general case given in Assumption 2.1, one can achieve all the conclusions by confining all the MAPs inside $B_{R_1}(0)$.

We now summarize some notation that will be used later. For $\phi(t) \in \mathbb{R}^n$ defined on $\Gamma_T = [0, T]$, we let $|\phi|^2 = \sum_{i=1}^n |\phi_i|^2$ and $|\phi|^2_{m,\Gamma_T} = \sum_{i=1}^n |\phi_i|^2_{m,\Gamma_T}$, where ϕ_i is the ith component of ϕ and $|\phi_i|^2_{m,\Gamma_T} = \int_{\Gamma_T} |\phi_i^{(m)}|^2\, dt$. We let $\|\phi\|^2_{m,\Gamma_T} = \sum_{i=1}^n \|\phi_i\|^2_{m,\Gamma_T}$, where $\|\phi_i\|^2_{m,\Gamma_T} = \sum_{k\le m}\int_{\Gamma_T} |\phi_i^{(k)}|^2\, dt$. For $f(t), g(t) \in \mathbb{R}^n$ defined on Γ_T, we define the inner products $\langle f, g\rangle = \sum_{i=1}^n f_i g_i$ and $\langle f, g\rangle_{\Gamma_T} = \int_{\Gamma_T} (\sum_{i=1}^n f_i g_i)\, dt$.

3. A reformulation of S_T.

We start with a necessary condition given by Maupertuis' principle of least action for the minimizer (T^*, ϕ^*) of Problem II.

Lemma 3.1 ([14]). *Let* (T^*, ϕ^*) *be the minimizer of Problem* II. *Then* ϕ^* *is located on the surface* $H(\phi, \frac{\partial L}{\partial \phi'}) = 0$, *where* H *is the Hamiltonian given by the Legendre transform of* $L(\phi, \phi') := \frac{1}{2}|\phi' - b(\phi)|^2$. *More specifically, for* (1.1),

$$H\left(\phi, \frac{\partial L}{\partial \phi'}\right) = 0 \quad \Longleftrightarrow \quad |\phi'(t)| = |b(\phi(t))| \quad \forall\, t. \tag{3.1}$$

We will call (3.1) the zero-Hamiltonian constraint in this paper. The zero-Hamiltonian constraint defines a nonlinear mapping between the arc length of the geometrically fixed lines on surface $H = 0$ and time t (see section 4.3.1 for more details). We instead consider a linear time scaling on Γ_T, which is simpler and more flexible for numerical approximation. For any given transition path ϕ and a fixed T, we consider the change of variable $s = t/T \in [0, 1] = \Gamma_1$. Let $\phi(t) = \phi(sT) =: \bar{\phi}(s)$. Then $\bar{\phi}'(s) = \phi'(t)T$, and we rewrite the action functional as

$$S_T(\phi(t)) = S_T(\bar{\phi}(s)) = \frac{T}{2}\int_0^1 \left|T^{-1}\bar{\phi}'(s) - b(\bar{\phi}(s))\right|^2 ds =: S(T, \bar{\phi}). \tag{3.2}$$

LEMMA 3.2. *For any given transition path ϕ, we have*

$$\hat{S}(\bar{\phi}) := S(\hat{T}(\bar{\phi}), \bar{\phi}) = \inf_{T\in\mathbb{R}^+} S(T, \bar{\phi}) \tag{3.3}$$

if $\hat{T}(\bar{\phi}) < \infty$, where

$$\hat{T}(\bar{\phi}) = \frac{|\bar{\phi}'|_{0,\Gamma_1}}{|b(\bar{\phi})|_{0,\Gamma_1}}. \tag{3.4}$$

Proof. It is easy to verify that the functional $\hat{T}(\bar{\phi})$ is nothing but the unique solution of the optimality condition $\partial_T S(T, \bar{\phi}) = 0$. ◻

COROLLARY 3.3. *Let (T^*, ϕ^*) be the minimizer of Problem* II. *If $T^* < \infty$, we have $T^* = \hat{T}(\bar{\phi}^*)$, where $\bar{\phi}^*(s):=\phi^*(sT^*)$.*

Proof. From the zero-Hamiltonian constraint (3.1) and the definition of $\bar{\phi}$, we have

$$|(\bar{\phi}^*)'| = |(\phi^*)'|T^* = |b(\phi^*)|T^* = |b(\bar{\phi}^*)|T^*.$$

Integrating both sides on Γ_1, we have the conclusion. ◻

For any absolutely continuous path ϕ, it is shown in Theorem 5.6.3 in [5] that S_T can be written as

$$S_T(\phi) = \begin{cases} S_T(\phi), & \phi \in H^1(\Gamma_T; \mathbb{R}^n), \\ \infty & \text{otherwise.} \end{cases} \tag{3.5}$$

This means that we can seek the MAP in the Sobolev space $H^1(\Gamma_T; \mathbb{R}^n)$. From now on, we will use $H^1(\Gamma_T)$ to indicate $H^1(\Gamma_T; \mathbb{R}^n)$ if no ambiguity arises. The same rule will be applied to other spaces such as $H_0^1(\Gamma; \mathbb{R}^n)$ and $L^2(\Gamma; \mathbb{R}^n)$.

We define the following two admissible sets consisting of transition paths:

$$\mathcal{A}_T = \{\phi \in H^1(\Gamma_T) : \phi(0) = 0,\, \phi(T) = x\}, \tag{3.6}$$

$$\mathcal{A}_1 = \{\bar{\phi} \in H^1(\Gamma_1) : \bar{\phi}(0) = 0,\, \bar{\phi}(1) = x\}, \tag{3.7}$$

where we let $x_1 = 0$ and $x_2 = x$ just for convenience.

LEMMA 3.4. *If $T^* < \infty$, we have*

$$S_{T^*}(\phi^*) = \hat{S}(\bar{\phi}^*) = \inf_{\bar{\phi}\in\mathcal{A}_1} \hat{S}(\bar{\phi}) \tag{3.8}$$

and $T^* = \hat{T}(\bar{\phi}^*)$ (see (3.4)), where $\phi^*(t) = \bar{\phi}^*(t/T^*)$ (or $\bar{\phi}^*(s) = \phi^*(sT^*)$).

Proof. If (T^*, ϕ^*) is a minimizer of $S_T(\phi)$ and $T^* < \infty$, then

$$S_{T^*}(\phi^*) = \inf_{T\in\mathbb{R}^+} \inf_{\phi\in\mathcal{A}_T} S_T(\phi) = \inf_{\bar\phi\in\mathcal{A}_1} \hat S(\bar\phi) \le \hat S(\bar\phi^*)$$

and

$$\hat S(\bar\phi^*) = \inf_{T\in\mathbb{R}^+} S(T, \bar\phi^*) = \inf_{T\in\mathbb{R}^+} S_T(\phi^*) \le S_{T^*}(\phi^*).$$

Thus, $S_{T^*}(\phi^*) = S(T^*, \bar\phi^*) = \hat S(\bar\phi^*)$; that is, $\bar\phi^*$ is a minimizer of $\hat S(\bar\phi)$ for $\bar\phi \in \mathcal{A}_1$, and $T^* = \hat T(\bar\phi^*)$ from Corollary 3.3.

Conversely, if $\bar\phi^*$ is a minimizer of $\hat S(\bar\phi)$, we let $T^* = \hat T(\bar\phi^*)$ and $\phi^*(t) = \bar\phi^*(\frac{t}{T^*})$ for $t \in [0, T^*]$. We have

$$S_{T^*}(\phi^*) = S(\hat T(\bar\phi^*), \bar\phi^*) = \hat S(\bar\phi^*) = \inf_{\bar\phi\in\mathcal{A}_1} \hat S(\bar\phi) = \inf_{T\in\mathbb{R}^+} \inf_{\phi\in\mathcal{A}_T} S_T(\phi)$$

when $T^* < \infty$. Then (T^*, ϕ^*) is a minimizer of $S_T(\phi)$. So the minimizers of $\hat S(\bar\phi)$ and $S_T(\phi)$ have a one-to-one correspondence when the optimal integral time is finite. ∎

Lemma 3.4 shows that for a finite T^* we can use (3.8) instead of Problem II to approximate the quasi-potential such that the optimization parameter T is removed, and we obtain a new problem

$$\hat S(\bar\phi^*) = \inf_{\substack{\bar\phi(0)=x_1,\\ \bar\phi(1)=x_2}} \hat S(\bar\phi) \tag{3.9}$$

that is equivalent to Problem II.

4. Finite element discretization of Problems I and II. The numerical method to approximate Problems I and II is usually called the minimum action method (MAM) [7]. Many versions of MAM have been developed, where the action functional is discretized by either a finite difference method or a finite element method. In this work, we consider the finite element discretization of $S_T(\phi)$ and focus on the convergence of the finite element approximation of the minimizer.

Let $\mathcal{T}_h$ and $\overline{\mathcal{T}}_h$ be partitions of Γ_T and Γ_1, respectively. We define the following approximation spaces given by linear finite elements:

$$\mathcal{B}_h = \{\phi_h \in \mathcal{A}_T : \phi_h|_I \text{ is affine for each } I \in \mathcal{T}_h\},$$
$$\overline{\mathcal{B}}_h = \{\bar\phi_h \in \mathcal{A}_1 : \bar\phi_h|_I \text{ is affine for each } I \in \overline{\mathcal{T}}_h\}.$$

For any h, we define the following discretized action functionals:

$$S_{T,h}(\phi_h) = \begin{cases} \frac{1}{2}\int_0^T |\phi_h' - b(\phi_h)|^2\, dt & \text{if } \phi_h \in \mathcal{B}_h, \\ \infty & \text{if } \phi_h \notin \mathcal{B}_h \end{cases} \tag{4.1}$$

and

$$\hat S_h(\bar\phi_h) = \begin{cases} \frac{\hat T(\bar\phi_h)}{2}\int_0^1 |\frac{1}{\hat T(\bar\phi_h)}\bar\phi_h' - b(\bar\phi_h)|^2\, dt & \text{if } \bar\phi_h \in \overline{\mathcal{B}}_h, \\ \infty & \text{if } \bar\phi_h \notin \overline{\mathcal{B}}_h. \end{cases} \tag{4.2}$$

We note that for a fixed integration time T, we can rewrite $S_T(\phi)$ as $\hat S(\bar\phi)$ by letting $T = \hat T$, such that Problem I can also be defined on Γ_1. Since we intend to use the reformulation $\hat S(\bar\phi)$ to deal with the parameter T in Problem II, we use Γ_T and Γ_1 to define Problems I and II, respectively, for clarity.

4.1. Problem I with a fixed T. For this case, our main results are summarized in the following theorem.

THEOREM 4.1. *For Problem* I *with a fixed T, we have*

$$\min_{\phi\in\mathcal{A}_T} S_T(\phi) = \lim_{h\to 0}\inf_{\phi_h\in\mathcal{B}_h} S_{T,h}(\phi_h),$$

namely, the minima of $S_{T,h}$ converge to the minimum of $S_T(\phi)$ as $h\to 0$. Moreover, if $\{\phi_h\}\subset\mathcal{B}_h$ is a sequence of minimizers of $S_{T,h}$, then there is a subsequence that converges weakly in $H^1(\Gamma_T)$ to some $\phi\in\mathcal{A}_T$, which is a minimizer of S_T.

The proof of this theorem will be split into two steps: (1) the existence of the minimizer of $S_T(\phi)$ in $\mathcal{A}_T$, and (2) Γ-convergence of $S_{T,h}$ to S_T as $h\to 0$.

4.1.1. Solution existence in $\mathcal{A}_T$. We search the minimizer of $S_T(\phi)$ in the admissible set $\mathcal{A}_T$. The solution existence is given by the following lemma.

LEMMA 4.2. *There exists at least one function $\phi^*\in\mathcal{A}_T$ such that*

$$S_T(\phi^*) = \min_{\phi\in\mathcal{A}_T} S_T(\phi).$$

Proof. We first establish the coerciveness of $S_T(\phi)=\frac{1}{2}\int_0^T|\phi'-b(\phi)|^2\,dt$. In order to do so, we define an auxiliary function g by

$$g(t)=\phi(t)-\int_0^t b(\phi(u))\,du.$$

Then $g'=\phi'-b(\phi)$ and $g(0)=0$. Since $b(x)$ is globally Lipschitz continuous, we have

$$\begin{aligned}|\phi'(t)| &\le |b(\phi(t))-b(0)|+|b(0)|+|g'|\\ &\le K|\phi|+|b(0)|+|g'(t)|\\ &\le K\int_0^t|\phi'(s)|\,ds+|b(0)|+|g'(t)|.\end{aligned}$$

By Gronwall's inequality, we have

$$|\phi'(t)|\le K\int_0^t(|b(0)|+|g'(s)|)e^{K(t-s)}\,ds+|b(0)|+|g'(t)|,$$

from which we obtain

$$|\phi|_{1,\Gamma_T}\le C_1|b(0)|^2+C_2|g|^2_{1,\Gamma_T},$$

where C_1 and C_2 are two positive constants depending on K and T. Thus, the action functional satisfies

$$S_T(\phi)=\frac{1}{2}|g|^2_{1,\Gamma_T}\ge\frac{1}{2}C_2^{-1}|\phi|^2_{1,\Gamma_T}-\frac{1}{2}C_1C_2^{-1}|b(0)|^2.$$

The coerciveness follows. On the other hand, the integrand $|\phi'-b(\phi)|^2$ is bounded below by 0 and convex in ϕ'. By Theorem 2 of [9, p. 448], $S_T(\phi)$ is weakly lower semicontinuous on $H^1(\Gamma_T)$.

For any minimizing sequence $\{\phi_k\}_{k=1}^\infty$, from the coerciveness, we have

$$\sup_k|\phi_k|_{1,\Gamma_T}<\infty.$$

Let $\phi_0 \in \mathcal{A}_T$ be any fixed function, e.g., the linear function on Γ_T from 0 to x. Then $\phi_k - \phi_0 \in H_0^1(\Gamma_T)$, and

$$\begin{aligned}|\phi_k|_{0,\Gamma_T} &\le |\phi_k - \phi_0|_{0,\Gamma_T} + |\phi_0|_{0,\Gamma_T}\\ &\le C_p|\phi_k - \phi_0|_{1,\Gamma_T} + |\phi_0|_{0,\Gamma_T} < \infty,\end{aligned}$$

by Poincaré's inequality. Thus $\{\phi_k\}_{k=1}^{\infty}$ is bounded in $H^1(\Gamma_T)$. Then there exists a subsequence $\{\phi_{k_j}\}_{j=1}^{\infty}$ converging weakly to some $\phi^* \in H^1(\Gamma_T)$ in $H^1(\Gamma_T)$, which means $\phi_{k_j} - \phi_0$ converges to $\phi^* - \phi_0$ weakly in $H_0^1(\Gamma_T)$. By Mazur's theorem [9], $H_0^1(\Gamma_T)$ is weakly closed. So $\phi^* - \phi_0 \in H_0^1(\Gamma_T)$, i.e., $\phi^* \in \mathcal{A}_T$.

Therefore, $S_T(\phi^*) \le \liminf_{j\to\infty} S_T(\phi_{k_j}) = \inf_{\phi\in\mathcal{A}_T} S_T(\phi)$. Since $\phi^* \in \mathcal{A}_T$, we reach the conclusion. ∎

4.1.2. Γ-convergence of $\boldsymbol{S_{T,h}}$. We first note the following simple property.

PROPERTY 4.3. *For any sequence $\{\phi_h\} \subset \mathcal{B}_h$ converging weakly to $\phi \in H^1(\Gamma_T)$, we have*

$$\lim_{h\to 0} |b(\phi_h) - b(\phi)|_{0,\Gamma_T} = 0.$$

Proof. Since ϕ_h converges weakly to ϕ in $H^1(\Gamma_T)$, $\phi_h \to \phi$ in $L^2(\Gamma_T)$; i.e., ϕ_h converges strongly to ϕ in the L^2 sense. By the Lipschitz continuity of b, we reach the conclusion. ∎

We now establish the Γ-convergence of $S_{T,h}$.

LEMMA 4.4 (Γ-convergence of $S_{T,h}$). *Let $\{\mathcal{T}_h\}$ be a sequence of finite element meshes with $h \to 0$. For every $\phi \in \mathcal{A}_T$, the following two properties hold:*

- *Lim-inf inequality: for every sequence $\{\phi_h\}$ converging weakly to ϕ in $H^1(\Gamma_T)$, we have*

$$S_T(\phi) \le \liminf_{h\to 0} S_{T,h}(\phi_h). \tag{4.3}$$

- *Lim-sup inequality: there exists a sequence $\{\phi_h\} \subset \mathcal{B}_h$ converging weakly to ϕ in $H^1(\Gamma_T)$, such that*

$$S_T(\phi) \ge \limsup_{h\to 0} S_{T,h}(\phi_h). \tag{4.4}$$

Proof. We first address the lim-inf inequality. We only need to consider a sequence $\{\phi_h\} \subset \mathcal{B}_h$, since otherwise, (4.3) is trivial by the definition of $S_{T,h}(\phi)$. Let $\{\phi_h\} \subset \mathcal{B}_h$ be an arbitrary sequence converging weakly to ϕ in $H^1(\Gamma_T)$. The action functional can be written as

$$\begin{aligned}&\int_0^T |\phi_h' - b(\phi_h)|^2\,dt\\ &= \int_0^T |\phi_h'|^2\,dt + \int_0^T |b(\phi_h)|^2\,dt - 2\int_0^T \langle \phi_h', b(\phi_h)\rangle\,dt = I_1 + I_2 + I_3.\end{aligned} \tag{4.5}$$

The functional defined by I_1 is obviously weakly lower semicontinuous in $H^1(\Gamma_T)$ since the integrand is convex with respect to ϕ'.

For I_2 in (4.5): Using Property 4.3, we have

$$\lim_{h\to 0} |b(\phi_h)|_{0,\Gamma_T} = |b(\phi)|_{0,\Gamma_T}.$$

For I_3 in (4.5): We have

$$\begin{aligned}
&\left|\int_0^T \langle \phi_h', b(\phi_h)\rangle\,dt - \int_0^T \langle \phi', b(\phi)\rangle\,dt\right| \\
&= \left|\int_0^T \langle \phi_h', b(\phi_h) - b(\phi)\rangle\,dt + \int_0^T \langle \phi_h' - \phi', b(\phi)\rangle\,dt\right| \\
&\leq |\phi_h|_{1,\Gamma_T} |b(\phi_h) - b(\phi)|_{0,\Gamma_T} + |\langle \phi_h' - \phi', b(\phi)\rangle_{\Gamma_T}|.
\end{aligned}$$

Using Property 4.3 and the fact that $\sup_h |\phi_h|_{1,\Gamma_T} < \infty$, we have that the first term of the above inequality converges to 0. Moreover, the second term also converges to 0 due to the weak convergence of ϕ_h to ϕ in $H^1(\Gamma_T)$. Thus,

$$\lim_{h\to 0} \int_0^T \langle \phi_h', b(\phi_h)\rangle\,dt = \int_0^T \langle \phi', b(\phi)\rangle\,dt.$$

Combining the results for I_1, I_2, and I_3, we obtain

$$\begin{aligned}
&\liminf_{h\to 0} \int_0^T |\phi_h' - b(\phi_h)|^2\,dt \\
&= \liminf_{h\to 0} \left[\int_0^T |\phi_h'|^2\,dt + \int_0^T |b(\phi_h)|^2\,dt - 2\int_0^T \langle \phi_h', b(\phi_h)\rangle\,dt\right] \\
&= \liminf_{h\to 0} \int_0^T |\phi_h'|^2\,dt + \lim_{h\to 0} \int_0^T |b(\phi_h)|^2\,dt - 2\lim_{h\to 0} \int_0^T \langle \phi_h', b(\phi_h)\rangle\,dt \\
&\geq \int_0^T |\phi'|^2\,dt + \int_0^T |b(\phi)|^2\,dt - 2\int_0^T \langle \phi', b(\phi)\rangle\,dt \\
&= \int_0^T |\phi' - b(\phi)|^2\,dt,
\end{aligned}$$

which yields the lim-inf inequality.

We now address the lim-sup inequality. Since $H^2(\Gamma_T)$ is dense in $H^1(\Gamma_T)$, for any $\phi \in H^1(\Gamma_T)$ and $\varepsilon > 0$, there exists a nonzero $u_\varepsilon \in H^2(\Gamma_T)$, such that $\|\phi - u_\varepsilon\|_{1,\Gamma_T} < \varepsilon$. We have

$$|\mathcal{I}_h u_\varepsilon - u_\varepsilon|_{1,\Gamma_T} \leq ch|u_\varepsilon|_{2,\Gamma_T} \leq c\varepsilon,$$

by letting

$$h = h(\varepsilon) = \min\left\{\frac{\varepsilon}{|u_\varepsilon|_{1,\Gamma_T}}, \frac{\varepsilon}{|u_\varepsilon|_{2,\Gamma_T}}, \varepsilon\right\},$$

where $\mathcal{I}_h$ is an interpolation operator defined by linear finite elements. Let $\phi_h = \mathcal{I}_h u_\varepsilon$. Then we have $\phi_h \in \mathcal{B}_h$, and

$$\begin{aligned}
|\phi_h - \phi|_{1,\Gamma_T} &\leq |\phi_h - u_\varepsilon|_{1,\Gamma_T} + |u_\varepsilon - \phi|_{1,\Gamma_T} \\
&= |\mathcal{I}_h u_\varepsilon - u_\varepsilon|_{1,\Gamma_T} + |u_\varepsilon - \phi|_{1,\Gamma_T} \\
&< c\varepsilon + \varepsilon \to 0
\end{aligned}$$

and

$$\begin{aligned}
|\phi_h - \phi|_{0,\Gamma_T} &\leq |\phi_h - u_\varepsilon|_{0,\Gamma_T} + |u_\varepsilon - \phi|_{0,\Gamma_T} \\
&= |\mathcal{I}_h u_\varepsilon - u_\varepsilon|_{0,\Gamma_T} + |u_\varepsilon - \phi|_{0,\Gamma_T} \\
&\leq ch|u_\varepsilon|_{1,\Gamma_T} + \varepsilon \\
&< c\varepsilon + \varepsilon \to 0
\end{aligned}$$

as $\varepsilon \to 0$. So ϕ_h converges to ϕ in $H^1(\Gamma_T)$, and also converges weakly in $H^1(\Gamma_T)$. By Property 4.3, we know that $b(\phi_h) \to b(\phi)$ in $L_2(\Gamma_T)$. Thus,

$$\lim_{h\to 0} S_{T,h}(\phi_h) = \lim_{h\to 0} \frac{1}{2}|\phi_h' - b(\phi_h)|^2_{0,\Gamma_T} = S_T(\phi),$$

which yields the lim-sup equality. ∎

4.1.3. Proof of Theorem 4.1. With the solution existence and Γ-convergence being proved, we need only the equicoerciveness of $S_{T,h}$ for the final conclusion. For any $\phi_h \in \mathcal{B}_h$, we have $S_{T,h}(\phi_h) = S_T(\phi_h)$. Then the equicoerciveness of $S_{T,h}$ in $\mathcal{B}_h$ follows from the coerciveness of $S_T(\phi_h)$ restricted to $\mathcal{B}_h \subset \mathcal{A}_T$ (see the first step in the proof of Lemma 4.2).

4.2. Problem II with a finite T^*. For this case, we consider the reformulation of S_T given in section 3. From Lemma 3.4, we know that Problem II with a finite T^* is equivalent to minimizing $\hat{S}$ in $\mathcal{A}_1$ (see (3.8)). Our main results are summarized in the following theorem.

THEOREM 4.5. *For Problem* II *with a finite T^*, we have*

$$\min_{\bar{\phi}\in\mathcal{A}_1} \hat{S}(\bar{\phi}) = \lim_{h\to 0} \inf_{\bar{\phi}_h\in\overline{\mathcal{B}}_h} \hat{S}_h(\bar{\phi}_h);$$

namely, the minima of $\hat{S}_h$ converge to the minimum of $\hat{S}$ as $h \to 0$. Moreover, if $\{\bar{\phi}_h\} \subset \overline{\mathcal{B}}_h$ is a sequence of minimizers of $\hat{S}_h$, then there is a subsequence that converges weakly in $H^1(\Gamma_1)$ to some $\bar{\phi} \in \mathcal{A}_1$, which is a minimizer of $\hat{S}$.

Similarly to Problem I with a fixed T, we split the proof of this theorem into two steps: (1) the existence of the minimizer of $\hat{S}(\bar{\phi})$ in $\mathcal{A}_1$, and (2) Γ-convergence of $\hat{S}_h$ to $\hat{S}$ as $h \to 0$.

4.2.1. Solution existence in $\mathcal{A}_1$. We start from the following property of the functional $\hat{T}$.

PROPERTY 4.6. *There exists a constant $C_{\hat{T}} > 0$ such that*

$$\hat{T}(\bar{\phi}) \geq C_{\hat{T}} \tag{4.6}$$

for any $\bar{\phi} \in \mathcal{A}_1$.

Proof. For any $\bar{\phi} \in \mathcal{A}_1$, let $\bar{\phi} = \bar{\phi}_0 + \bar{\phi}_L$, where $\bar{\phi}_0 \in H^1_0(\Gamma_1)$ and $\bar{\phi}_L(s) = xs$, $s \in [0,1]$, is a linear function connecting 0 and x. We have

$$\begin{aligned}
\hat{T}(\bar{\phi}) &= \frac{|\bar{\phi}_0' + x|_{0,\Gamma_1}}{|b(\bar{\phi}_0 + \bar{\phi}_L)|_{0,\Gamma_1}} \\
&\geq \frac{|\bar{\phi}_0' + x|_{0,\Gamma_1}}{|b(\bar{\phi}_0 + \bar{\phi}_L) - b(\bar{\phi}_L)|_{0,\Gamma_1} + |b(\bar{\phi}_L)|_{0,\Gamma_1}} \\
&\geq \frac{|\bar{\phi}_0' + x|_{0,\Gamma_1}}{K|\bar{\phi}_0|_{0,\Gamma_1} + |b(\bar{\phi}_L)|_{0,\Gamma_1}} \\
&\geq \frac{|\bar{\phi}_0' + x|_{0,\Gamma_1}}{KC_p|\bar{\phi}_0'|_{0,\Gamma_1} + |b(\bar{\phi}_L)|_{0,\Gamma_1}},
\end{aligned}$$

where C_p is the constant for Poincaré's inequality. Thus,

$$\begin{aligned}\hat{T}(\bar{\phi})^2 &\geq \frac{|\bar{\phi}_0' + x|^2_{0,\Gamma_1}}{2K^2C_p^2|\bar{\phi}_0'|^2_{0,\Gamma_1} + 2|b(\bar{\phi}_L)|^2_{0,\Gamma_1}} \\ &= \frac{|\bar{\phi}_0' + x|^2_{0,\Gamma_1}}{C_1|\bar{\phi}_0'|^2_{0,\Gamma_1} + C_2} \\ &=: J(\bar{\phi}_0) > 0,\end{aligned}$$

where $C_1 = 2K^2C_p^2 > 0$ and $C_2 = 2|b(\bar{\phi}_L)|^2_{0,\Gamma_1} > 0$.

Let $\delta\bar{\phi} \in H_0^1(\Gamma_1)$ be a perturbation function with $\delta\bar{\phi}(0) = \delta\bar{\phi}(1) = 0$. We have

$$\begin{aligned}&J(\bar{\phi}_0 + \delta\bar{\phi}) - J(\bar{\phi}_0) \\ =&\frac{|\bar{\phi}_0' + x + \delta\bar{\phi}'|^2_{0,\Gamma_1}}{C_1|\bar{\phi}_0' + \delta\bar{\phi}'|^2_{0,\Gamma_1} + C_2} - \frac{|\bar{\phi}_0' + x|^2_{0,\Gamma_1}}{C_1|\bar{\phi}_0'|^2_{0,\Gamma_1} + C_2} \\ =&\frac{|\bar{\phi}_0' + x + \delta\bar{\phi}'|^2_{0,\Gamma_1}(C_1|\bar{\phi}_0'|^2_{0,\Gamma_1} + C_2) - |\bar{\phi}_0' + x|^2_{0,\Gamma_1}(C_1|\bar{\phi}_0' + \delta\bar{\phi}'|^2_{0,\Gamma_1} + C_2)}{(C_1|\bar{\phi}_0' + \delta\bar{\phi}'|^2_{0,\Gamma_1} + C_2)(C_1|\bar{\phi}_0'|^2_{0,\Gamma_1} + C_2)} \\ =&\frac{2\langle\bar{\phi}_0' + x, \delta\bar{\phi}'\rangle_{\Gamma_1}(C_1|\bar{\phi}_0'|^2_{0,\Gamma_1} + C_2) - 2C_1\langle\bar{\phi}_0', \delta\bar{\phi}'\rangle_{\Gamma_1}|\bar{\phi}_0' + x|^2_{0,\Gamma_1}}{(C_1|\bar{\phi}_0'|^2_{0,\Gamma_1} + C_2)^2} + R(\bar{\phi}_0', x, \delta\bar{\phi}'),\end{aligned}$$

where R is the remainder term of $O(|\delta\bar{\phi}|^2_{1,\Gamma_1})$.

We then have the first-order variation of J as

$$\delta J = \frac{2\langle\bar{\phi}_0', \delta\bar{\phi}'\rangle_{\Gamma_1}(C_1|\bar{\phi}_0'|^2_{0,\Gamma_1} + C_2 - C_1|\bar{\phi}_0' + x|^2_{0,\Gamma_1})}{(C_1|\bar{\phi}_0'|^2_{0,\Gamma_1} + C_2)^2}.$$

The optimality condition $\delta J = 0$ yields two possible cases: $\bar{\phi}_0' = 0$ and $C_1|\bar{\phi}_0'|^2_{0,\Gamma_1} + C_2 = C_1|\bar{\phi}_0' + x|^2_{0,\Gamma_1}$. For the first case, $\bar{\phi}_0$ is a constant. But $\bar{\phi}_0 \in H_0^1(\Gamma_1)$, so $\bar{\phi}_0 = 0$. Then $J(0) = \frac{|x|^2}{C_2} > 0$. For the second case, $J(\bar{\phi}_0) = \frac{1}{C_1} > 0$. Thus,

$$\hat{T}^2(\bar{\phi}) \geq \min\left\{\frac{|x|^2}{C_2}, \frac{1}{C_1}\right\}.$$

More specifically,

$$\hat{T}(\bar{\phi}) \geq C_{\hat{T}} := \min\left\{\frac{|x|}{\sqrt{2}|b(\bar{\phi}_L)|^2_{0,\Gamma_1}}, \frac{1}{\sqrt{2}KC_p}\right\} > 0. \qquad \square$$

We search for the minimizer of $\hat{S}(\bar{\phi})$ in the admissible set $\mathcal{A}_1$. The solution existence is given by the following lemma.

LEMMA 4.7. *If the optimal integral time T^* for Problem* II *is finite, there exists at least one function $\phi^* \in \mathcal{A}_T$ such that*

$$S_{T^*}(\phi^*) = \min_{\substack{T\in\mathbb{R}^+,\\ \phi\in\mathcal{A}_T}} S_T(\phi) = \min_{\bar{\phi}\in\mathcal{A}_1} \hat{S}(\bar{\phi}).$$

Proof. We first establish the weakly lower semicontinuity of $\hat{S}(\bar{\phi})$ in $H^1(\Gamma_1)$. Rewrite $\hat{S}(\bar{\phi})$ by substituting (3.4) to get

$$\begin{aligned}\hat{S}(\bar{\phi}) &= \frac{\hat{T}(\bar{\phi})}{2}\int_0^1 \left|\hat{T}^{-1}(\bar{\phi})\bar{\phi}' - b(\bar{\phi})\right|^2 dt \\ &= |\bar{\phi}'|_{0,\Gamma_1}|b(\bar{\phi})|_{0,\Gamma_1} - \langle \bar{\phi}', b(\bar{\phi})\rangle_{\Gamma_1}.\end{aligned}$$

For any sequence $\bar{\phi}_k$ converging weakly to $\bar{\phi}$ in $H^1(\Gamma_1)$, $\{\bar{\phi}'_k\}$ is bounded in $L^2(\Gamma_1)$ and $\bar{\phi}_k \to \bar{\phi}$ in $L^2(\Gamma_1)$. Coupling with the global Lipschitz continuity of b, we can obtain

$$\begin{aligned}\lim_{k\to\infty} |b(\bar{\phi}_k)|^2_{0,\Gamma_1} &= |b(\bar{\phi})|^2_{0,\Gamma_1}, \\ \lim_{k\to\infty} \langle \bar{\phi}'_k, b(\bar{\phi}_k)\rangle_{\Gamma_1} &= \langle \bar{\phi}', b(\bar{\phi})\rangle_{\Gamma_1}.\end{aligned}$$

The weakly lower semicontinuity of $|\bar{\phi}'|_{0,\Gamma_1}$ yields that

$$\liminf_{k\to\infty} |\bar{\phi}'_k|_{0,\Gamma_1} \geq |\bar{\phi}'|_{0,\Gamma_1}. \tag{4.7}$$

Combining the above results, we obtain

$$\begin{aligned}&\liminf_{k\to\infty} \hat{S}_k(\bar{\phi}_k) \\ &= \liminf_{k\to\infty} \left(|\bar{\phi}'_k|_{0,\Gamma_1}|b(\bar{\phi}_k)|_{0,\Gamma_1} - \langle \bar{\phi}'_k, b(\bar{\phi}_k)\rangle_{\Gamma_1}\right) \\ &= \liminf_{k\to\infty} |\bar{\phi}'_k|_{0,\Gamma_1}|b(\bar{\phi}_k)|_{0,\Gamma_1} - \lim_{k\to\infty}\langle \bar{\phi}'_k, b(\bar{\phi}_k)\rangle_{\Gamma_1} \\ &\geq |\bar{\phi}'|_{0,\Gamma_1}|b(\bar{\phi})|_{0,\Gamma_1} - \langle \bar{\phi}', b(\bar{\phi})\rangle_{\Gamma_1} \\ &= \hat{S}(\bar{\phi});\end{aligned}$$

that is, $\hat{S}(\bar{\phi})$ is weakly lower semicontinuous in $H^1(\Gamma_1)$.

We subsequently establish the coercivity of $\hat{S}(\bar{\phi})$. Since T^* is finite, there exists $M \in (T^*, \infty)$, such that

$$\inf_{\bar{\phi}\in\mathcal{A}_1} \hat{S}(\bar{\phi}) = \inf_{\substack{\bar{\phi}\in\mathcal{A}_1,\\ \hat{T}(\bar{\phi})<M}} \hat{S}(\bar{\phi}).$$

In fact, by Lemma 3.4, a minimizing sequence $\{\bar{\phi}_k\}$ of $\hat{S}(\bar{\phi})$ defines a minimizing sequence $\{(\hat{T}(\bar{\phi}_k), \bar{\phi}_k)\}$ of $S(T, \bar{\phi})$, which also corresponds to a minimizing sequence of $S_T(\phi)$. The assumption of $T^* < \infty$ allows us to add the condition that $\sup_k \hat{T}(\bar{\phi}_k) < M$. Otherwise, $\hat{T}(\bar{\phi}_k)$ must go to infinity. The continuity of $S(T, \bar{\phi})$ with respect to T yields that $T^* = \infty$, which contradicts our assumption that $T^* < \infty$. Now, let $\hat{T}^{-1}(\bar{\phi})\bar{\phi}'(s) - b(\bar{\phi}(s)) = \bar{g}'(s)$. Then for any $\bar{\phi} \in \mathcal{A}_1$ with $\hat{T}(\bar{\phi}) < M$,

$$\begin{aligned}|\bar{\phi}'| &\leq |\hat{T}(\bar{\phi})||b(\bar{\phi})| + |\hat{T}(\bar{\phi})||g'| \\ &\leq M|b(\bar{\phi})| + M|\bar{g}'| \\ &\leq MK|\bar{\phi}| + M|b(0)| + M|\bar{g}'| \\ &\leq MK\int_0^s |\bar{\phi}'(u)|\, du + M|b(0)| + M|\bar{g}'|.\end{aligned}$$

By Gronwall's inequality, we have

$$|\bar{\phi}'(s)| \leq \int_0^s M^2K(|\bar{g}'(u)| + |b(0)|)e^{KM(s-u)}\, du + M|b(0)| + M|\bar{g}'(s)|,$$

which yields

$$|\bar{\phi}'|_{0,\Gamma_1}^2 \le C_1|b(0)|^2 + C_2|\bar{g}'|_{0,\Gamma_1}^2, \tag{4.8}$$

where $C_1, C_2 \in (0,\infty)$ depend only on M and K. Thus,

$$\begin{aligned}
\hat{S}(\bar{\phi}) &= \frac{\hat{T}(\bar{\phi})}{2}\int_0^1 \left|\hat{T}^{-1}(\bar{\phi})\bar{\phi}'(s) - b(\bar{\phi}(s))\right|^2 ds \\
&= \frac{\hat{T}(\bar{\phi})}{2}|\bar{g}'|_{0,\Gamma_1}^2 \\
&\ge \frac{C_{\hat{T}}}{2}\left(\frac{1}{C_2}|\bar{\phi}'|_{0,\Gamma_1}^2 - \frac{C_1}{C_2}|b(0)|^2\right),
\end{aligned}$$

where we used Property 4.6 in the last step. This is the coercivity.

For any minimizing sequence $\{\bar{\phi}_k\}_{k=1}^\infty$ of $\hat{S}(\bar{\phi})$, we have

$$\sup_k |\bar{\phi}_k'|_{0,\Gamma_1} \le \frac{2C_1}{C_T}|b(0)|^2 + \frac{2C_2}{C_T}\sup_k\{\hat{S}(\bar{\phi}_k)\} < \infty.$$

Let $\bar{\phi}_0 \in \mathcal{A}_1$. Then

$$\begin{aligned}
|\bar{\phi}_k|_{0,\Gamma_1} &\le |\bar{\phi}_k - \bar{\phi}_0|_{0,\Gamma_1} + |\bar{\phi}_0|_{0,\Gamma_1} \\
&\le C_p|\bar{\phi}_k' - \bar{\phi}_0'|_{0,\Gamma_1} + |\bar{\phi}_0|_{0,\Gamma_1} < \infty
\end{aligned}$$

by Poincaré's inequality. Thus, $\{\bar{\phi}_k\}_{k=1}^\infty$ is bounded in $H^1(\Gamma_1)$. Then there is a subsequence $\{\bar{\phi}_{k_j}\}_{j=1}^\infty$ converging to some $\bar{\phi}^* \in H^1(\Gamma_1)$ weakly in $H^1(\Gamma_1)$. So $\bar{\phi}_{k_j} - \bar{\phi}_0$ converges weakly to $\bar{\phi}^* - \bar{\phi}_0$ in $H_0^1(\Gamma_1)$. By Mazur's theorem, $H_0^1(\Gamma_1)$ is weakly closed. So $\bar{\phi}^* - \bar{\phi}_0 \in H_0^1(\Gamma_1)$, and $\bar{\phi}^* \in \mathcal{A}_1$. By Lemma 3.4, $\phi^* \in \mathcal{A}_T$ corresponding to $\bar{\phi}^* \in \mathcal{A}_1$ is a minimizer of $S_T(\phi)$, and $T^* = \hat{T}(\bar{\phi}^*)$. ∎

4.2.2. Γ-convergence of $\hat{S}_h$. The Γ-convergence of $\hat{S}_h$ with respect to parameter h is established in the following lemma.

LEMMA 4.8 (Γ-convergence of $\hat{S}_h$). *Let $\{\mathcal{T}_h\}$ be a sequence of finite element meshes. For every $\bar{\phi} \in \mathcal{A}_1$, the following two properties hold:*

- *Lim-inf inequality: for every sequence $\{\bar{\phi}_h\}$ converging weakly to $\bar{\phi}$ in $H^1(\Gamma_1)$, we have*

$$\hat{S}(\bar{\phi}) \le \liminf_{h\to 0} \hat{S}_h(\bar{\phi}_h). \tag{4.9}$$

- *Lim-sup inequality: there exists a sequence $\{\bar{\phi}_h\} \subset \hat{\mathcal{B}}_h$ converging weakly to $\bar{\phi}$ in $H^1(\Gamma_1)$, such that*

$$\hat{S}(\bar{\phi}) \ge \limsup_{h\to 0} \hat{S}_h(\bar{\phi}_h). \tag{4.10}$$

Proof. We first address the lim-inf inequality. We only consider sequence $\{\bar{\phi}_h\} \subset \mathcal{B}_h$; otherwise, the inequality is trivial. Similarly to the proof of Lemma 4.7, rewrite the discretized functional as

$$\begin{aligned}
\hat{S}_h(\bar{\phi}_h) &= \frac{\hat{T}(\bar{\phi}_h)}{2}\int_0^1 \left|\hat{T}^{-1}(\bar{\phi}_h)\bar{\phi}_h' - b(\bar{\phi}_h)\right|^2 dt \\
&= |\bar{\phi}_h'|_{0,\Gamma_1}|b(\bar{\phi}_h)|_{0,\Gamma_1} - \langle\bar{\phi}_h', b(\bar{\phi}_h)\rangle_{\Gamma_1}.
\end{aligned}$$

By the same argument as in the proof of Lemma 4.4, we have

$$\begin{aligned}\liminf_{h\to 0}|\bar{\phi}_h'|_{0,\Gamma_1} &\geq |\bar{\phi}'|_{0,\Gamma_1},\\ \lim_{h\to 0}|b(\bar{\phi}_h)|_{0,\Gamma_1} &= |b(\bar{\phi})|_{0,\Gamma_1},\\ \lim_{h\to 0}\langle\bar{\phi}_h', b(\bar{\phi}_h)\rangle_{\Gamma_1} &= \langle\bar{\phi}', b(\bar{\phi})\rangle_{\Gamma_1}.\end{aligned}$$

Combining these results, we have the lim-inf inequality. The lim-sup inequality can be obtained by the same argument as in the proof of Lemma 4.4. ∎

4.2.3. Proof of Theorem 4.5. Similarly to the proof of Theorem 4.1, the only thing left is the verification of equicoerciveness of $\hat{S}_h(\bar{\phi}_h)$, which can be obtained directly from the coerciveness of $\hat{S}(\bar{\phi})$ restricted to $\bar{\mathcal{B}}_h \subset \mathcal{A}_1$ (see the second step in the proof of Lemma 4.7).

4.3. Problem II with an infinite T^*. When T^* is infinite, the integration domain becomes the whole real space, corresponding to a degenerate case of linear scaling. To remove the optimization parameter T, the zero-Hamiltonian constraint (3.1) can be considered under another assumption that the total arc length of ϕ^* is finite, which is the basic idea of the geometric MAM (gMAM) [14]. However, since the Jacobian of the transform between time and arc length variables will become singular at critical points, the numerical accuracy will deteriorate when unknown critical points exist along the MAP.

We will still work with the formulation with respect to time, which means that we need to use a large but finite integration time to deal with the case $T^* = \infty$. We discuss this case by considering a relatively simple scenario, but the numerical difficulties are reserved. Let $0 \in D$ be an asymptotically stable equilibrium point, D is contained in the basin of attraction of 0, and $\langle b(y), n(y)\rangle < 0$ for any $y \in \partial D$, where $n(y)$ is the exterior normal to the boundary ∂D. Then starting from any point in D, a trajectory of system (1.2) will converge to 0. We assume that the ending point x of Problem II is located on ∂D.

4.3.1. Escape from the equilibrium point. If we consider the change of variable in general, say $\alpha = \alpha(t)$, we have (see Lemma 3.1 in [11, Chapter 4])

$$S_T(\phi) \geq S(\tilde{\phi}) = \int_{\alpha(0)}^{\alpha(T)} (|\tilde{\phi}'||b| - \langle\tilde{\phi}', b\rangle)d\alpha, \tag{4.11}$$

where $\tilde{\phi}(\alpha) = \phi(t(\alpha))$, $\tilde{\phi}'$ is the derivative with respect to α, and the equality holds if the zero-Hamiltonian constraint (3.1) is satisfied. With respect to α, the zero-Hamiltonian constraint can be written as

$$|\tilde{\phi}'|\dot{\alpha}(t) = |b(\tilde{\phi})|, \tag{4.12}$$

from which we have

$$t = \int_0^{\alpha(t)} \frac{|\tilde{\phi}'|}{|b(\tilde{\phi})|}d\alpha. \tag{4.13}$$

If $|\tilde{\phi}'| \equiv$ const, the variable α is nothing but a rescaled arc length. Assuming that the length of the optimal curve is finite, we can rescale the total arc length to one, i.e., $\alpha(T) = 1$, which yields the gMAM [14].

We now look at any transition path $\tilde{\phi}(\alpha) = \phi(t(\alpha))$ that satisfies the zero-Hamiltonian constraint. Let α correspond to the arc length with $\tilde{\phi}(0) = 0$; then $|\tilde{\phi}'| = 1$. Let y be an arbitrary point on $\tilde{\phi}$. Then the integration time from 0 to y is

$$t = \int_0^{\alpha_y} \frac{1}{|b(\tilde{\phi})|} d\alpha,$$

where α_y is the arc length of the curve connecting 0 and y, i.e., the value of the arc length variable $\alpha(t)$ at point y. Note that if the end point y is in a small neighborhood of the equilibrium 0, the total arc length from 0 to y along $\bar{\phi}$ is small. However, from the fact that

$$|b(\tilde{\phi})| = |b(\tilde{\phi}) - b(0)| \leq K|\tilde{\phi}| \leq K\alpha,$$

we get

$$t = \int_0^{\alpha_y} \frac{1}{|b(\tilde{\phi})|} d\alpha \geq \int_0^{\alpha_y} \frac{1}{K\alpha} d\alpha = \infty,$$

as long as $\alpha_y > 0$. So $T^* = \infty$, because 0 is a critical point.

For clarity, we include the starting and ending points of the transition path in some notation. Let $\phi^*_{y,x}$ indicate the minimizer of Problem II with starting point y and ending point x, and let $T^*_{y,x}$ be the corresponding optimal integration time. We have, for any y on $\phi^*_{0,x}$, $T^*_{0,y} = \infty$ and $T^*_{y,x} < \infty$ for the exit problem as long as $\phi^*_{y,x}$ has a finite length.

4.3.2. Minimizing sequence for $\hat{S}(\phi)$. Let $\phi^L_{0,y} = yt$ be the linear function connecting 0 and y in one time unit $T = 1$. Then

$$\begin{aligned} S_{T^*_{0,y}}(\phi^*_{0,y}) \leq S_T(\phi^L_{0,y}) &= \frac{1}{2}\int_0^1 |y - b(yt)|^2 \, dt \\ &\leq \int_0^1 (|y|^2 + K^2|y|^2t^2)\, dt \leq C(K)\rho^2, \end{aligned}$$

where $|y| \leq \rho$. Although $T^*_{0,y} = \infty$ for any finite ρ, the action $S_{T^*_{0,y}}(\phi^*_{0,y})$ decreases to zero with respect to ρ. We consider a sequence of optimization problems

$$\hat{S}(\bar{\phi}^{*,n}_{0,x}) = \inf_{\substack{\hat{T}(\bar{\phi})\leq n,\\ \bar{\phi}\in\mathcal{A}_1}} \hat{S}(\bar{\phi}), \quad n = 1, 2, 3, \ldots, \tag{4.14}$$

generated by the constraint $\hat{T}(\bar{\phi}) \leq n$. We have the following.

LEMMA 4.9. $\{\bar{\phi}^{*,n}_{0,x}\}_{n=1}^{\infty}$ *is a minimizing sequence of* (3.9).

Proof. First, $\hat{S}(\phi^{*,n}_{0,x})$ is decreasing as n increases. Pick one ρ such that $x \notin B_\rho(0)$, and consider a sequence of $\rho_k = 2^{-k}\rho$, $k = 1, 2, \ldots$. Let y_k be the first intersection point of $\phi^*_{0,x}$ and $B_{\rho_k}(0)$ when traveling along $\phi^*_{0,x}$ from x to 0; thus $|y_k| = \rho_k$. The optimal transition time $T^*_{y_k,x} < \infty$. We construct a path from 0 to x as follows:

$$\phi_k = \begin{cases} \phi^L_{0,y_k}, t \in [-T^*_{y_k,x} - 1, -T^*_{y_k,x}], \\ \phi^*_{y_k,x}, t \in [-T^*_{y_k,x}, 0]. \end{cases}$$

Due to the additivity, we know that $\phi^*_{y_k,x}$ is located on $\phi^*_{0,x}$ since $y_k \in \phi^*_{0,x}$. Then $\{(T_k = T^*_{y_k,x} + 1, \phi_k)\}$ is a minimizing sequence as ρ_k decreases, and

$$S_{T_k}(\phi_k) \leq S_{T^*_{0,x}}(\phi^*_{0,x}) + C(K)\rho_k^2.$$

Consider $n = \lceil T_k \rceil$. We have

$$\hat{S}(\phi_{0,x}^{*,n}) \le S_{T_k}(\phi_k) \le S_{T_{0,x}^*}(\phi_{0,x}^*) + C(K)\rho_k^2,$$

where the first inequality is because $\hat{T}(\phi_k)$ is, in general, not equal to T_k. We then reach the conclusion. ∎

When $T^* = \infty$, we have $\hat{T}(\bar{\phi}) \to \infty$ as $\bar{\phi}$ gets close to the minimizer, implying that $|\bar{\phi}'|_{0,\Gamma_1} \to \infty$. Thus for this case, we cannot study the convergence in $H^1(\Gamma_1)$. A larger space is needed, i.e., the space consisting of absolutely continuous functions. So we use $\bar{C}_{x_1}^{x_2}(0,T)$, the space of absolutely continuous functions connecting x_1 and x_2 on $[0,T]$ with $0 < T \le \infty$. To prove the convergence of the minimizing sequence in Lemma 4.9, we use the following lemma, which is Proposition 2.1 proved in [14].

LEMMA 4.10. *Assume that the sequence* $((T_k, \phi_k))_{k\in\mathbb{N}}$ *with* $T_k > 0$ *and* $\phi_k \in \bar{C}_{x_1}^{x_2}(0,T_k)$ *for every* $k \in \mathbb{N}$ *is a minimizing sequence of* (2.2) *and that the lengths of the curves of* ϕ_k *are uniformly bounded, i.e.,*

$$\lim_{k\to\infty} S_{T_k}(\phi_k) = V(x_1,x_2) \quad \textit{and} \quad \sup_{k\in\mathbb{N}} \int_0^{T_k} |\dot{\phi}_k(t)|\,dt < \infty.$$

Then the action functional $\hat{S}$ *has a minimizer* φ^*, *and for some subsequence* $(\phi_{k_l})_{l\in\mathbb{N}}$ *we have that*

$$\lim_{l\to\infty} d(\phi_{k_l}, \varphi^*) = 0,$$

where d *denotes the Fréchet distance.*

THEOREM 4.11. *Assume that the lengths of the curves* $\phi_{0,x}^{*,n}$ *are uniformly bounded. Then there exists a subsequence* $\phi_{0,x}^{*,n_l}$ *that converges to a minimizer* $\phi^* \in \bar{C}_0^x(0,T)$ *with respect to the Fréchet distance.*

Proof. By Lemma 3.4, we have a one-to-one correspondence between $\{\bar{\phi}_{0,x}^{*,n}\}_{n=1}^\infty$ and $\{\phi_{0,x}^{*,n}\}_{n=1}^\infty$. So from Lemma 4.9, we know that $\{(n, \phi_{0,x}^{*,n})\}_{n=1}^\infty$ defines a minimizing sequence of Problem II. The convergence is a direct application of Lemma 4.10. ∎

Although we just constructed $\{\phi\}_{0,x}^{*,n}$ for an exit problem around the neighborhood of an asymptotically stable equilibrium, it is easy to see that the idea can be applied to a global transition, say both x_1 and x_2 are asymptotically stable equilibrium, as long as there exist finitely many critical points along the minimal action path. In (4.14), we introduced an extra constraint $\hat{T}(\bar{\phi}) \le n$, which implies that the infimum may be reached at the boundary $\hat{T}(\bar{\phi}) = n$. From the optimization point of view, such a box-type constraint is not favorable. Next, we will show that this constraint is not needed for the discrete problem.

4.3.3. Remove the constraint $\hat{T}(\bar{\phi}) \le n$ for a discrete problem. The key observation is as follows.

LEMMA 4.12. *If* $\bar{\phi}_h^*$ *is the minimizer of* $\hat{S}_h(\bar{\phi}_h)$ *over* $\overline{\mathcal{B}}_h$, *then* $\hat{T}(\bar{\phi}_h^*) \le C_h < \infty$ *for any given* h.

Proof. We argue by contradiction. Note that

$$\hat{T}^2(\bar{\phi}_h^*) = \frac{|(\bar{\phi}_h^*)'|_{0,\Gamma_1}^2}{|b(\bar{\phi}_h^*)|_{0,\Gamma_1}^2} \le C \frac{|\bar{\phi}_h^*|_{0,\Gamma_1}^2}{|b(\bar{\phi}_h^*)|_{0,\Gamma_1}^2},$$

where the last inequality is from the inverse inequality of finite element discretization and the constant C depends only on the mesh [3]. If $\hat{T}(\bar{\phi}_h^*) = \infty$, we have two possible cases: $|b(\bar\phi_h^*)|_{0,\Gamma_1} = 0$ or $|\bar\phi_h^*|_{0,\Gamma_1} = \infty$. The first case implies that $b(\bar\phi_h^*(s)) = 0$ for all $s \in \Gamma_1$, which contradicts statement (3) of Assumption 2.1. The second case implies that $\bar\phi_h^*$ must go to infinity somewhere due to the continuity, which contradicts Lemma 2.2. $\square$

Lemma 4.12 means that for a discrete problem the constraint $\hat T(\bar\phi) \le n$ in (4.14) is not necessary in the sense that there always exists a number n such that $\hat T(\bar\phi_h^*) < n$. We can then consider a sequence $\{\overline{\mathcal{T}}_h\}$ of finite element meshes and treat the minimization of $\hat S_h(\bar\phi_h)$ in exactly the same way as in the case that T^* is finite. Simply speaking, $\{(\hat T(\bar\phi_h^*), \bar\phi_h^*)\}$ defines a minimizing sequence as $h \to 0$ regardless of whether T^* is finite or infinite. The only difference between $T^* < \infty$ and $T^* = \infty$ is that we address the convergence of $\bar\phi_h^*$ in $H^1(\Gamma_1)$ for $T^* < \infty$ and in $\bar C_{x_1}^{x_2}$ for $T^* = \infty$.

4.3.4. The efficiency of $\{(\hat T(\bar\phi_h^*), \bar\phi_h^*)\}$. The E-L equation associated with $\hat S(\phi)$ is

$$\hat T^{-2}(\bar\phi)\bar\phi'' + \hat T^{-1}(\bar\phi)\left((\nabla_{\bar\phi} b)^{\mathsf T} - \nabla_{\bar\phi} b\right)\bar\phi' - (\nabla_{\bar\phi} b)^{\mathsf T} b = 0. \tag{4.15}$$

For a fixed T, the E-L equation associated with $S_T(\phi)$ is the same as (4.15) except that we need to replace $\hat T(\phi)$ with T [22]. If $T^* = \infty$, $\hat T(\bar\phi_h^*) \to \infty$ as $h \to 0$, which means that the E-L equation (4.15) eventually becomes degenerate. When h is small, $\hat T(\phi_h^*)$ is finite but large. Equation (4.15) can be regarded as a singularly perturbed problem, which implies the possible existence of boundary/internal layers. Thus the minimizing sequence given by a uniform refinement $\overline{\mathcal{T}}_h$ of Γ_1 may not be effective.

Consider a transition from a stable fixed point to a saddle point without any other critical points on the minimal transition path. The dynamics is slow around the critical points and fast elsewhere, which means that for the approximation given by a fixed large T, the path will be mainly captured in a subinterval $[a, b] \in \Gamma_1$ with $|b - a| \sim O(T^{-1})$ with respect to the scaled time $s = t/T$. Then an effective $\overline{\mathcal{T}}_h$ has a fine mesh for $[a, b]$ and a coarse mesh for $[0, a] \cup [b, 1]$. Currently, there exist two techniques to achieve an effective nonuniform discretization $\overline{\mathcal{T}}_h$:

(1) *Moving mesh technique.* Starting from a fine uniform discretization, the grid points will be redistributed such that more grid points will be moved from the region of slow dynamics to the region of fast dynamics [31, 20]. This procedure needs to be iterated until the optimal nonuniform mesh is reached with respect to a certain criterion for the redistribution of grids.

(2) *Adaptive finite element method.* Starting from a coarse uniform mesh, $\overline{\mathcal{T}}_h$ will be refined adaptively such that more elements will be put into the region of fast dynamics and fewer elements into the region of slow dynamics [22, 26]. Numerical experiments have shown that both techniques can recover the optimal convergence rate with respect to the number of degrees of freedom.

5. A priori error estimate for a linear ODE system. In this section we apply our strategy to a linear ODE system with $b(x) = -Ax$, where A is an SPD matrix. Then $x = 0$ is a global attractor. The E-L equation associated with $\hat S(\bar\phi)$ becomes

$$-\hat T^{-2}(\bar\phi)\bar\phi'' + A^2\bar\phi = 0, \tag{5.1}$$

which is a nonlocal elliptic problem of Kirchhoff type. For Problem I with a fixed T, i.e., $\hat T(\phi) = T$, (5.1) becomes a standard diffusion-reaction equation.

Let $\bar\phi^* = \bar\phi_0^* + \phi_L \in \mathcal{A}_1$ be the minimizer of $\hat S(\bar\phi)$, and $\bar\phi_h^* = \bar\phi_{h,0}^* + \phi_L \in \overline{\mathcal{B}}_h$ the minimizer of $\hat S_h(\bar\phi_h)$, where $\phi_L = x_1 + (x_2 - x_1)s$ is a linear function connecting x_1

and x_2 on Γ_1. Let

$$V_h = \{v\colon v|_I \text{ is affine } \forall\, I \in \overline{\mathcal{T}}_h,\ v(0) = v(1) = 0\} \subset H_0^1(\Gamma_1).$$

For a fixed T, (5.1) has a unique solution, and the standard argument shows that

$$\left|\bar\phi^* - \bar\phi_h^*\right|_{1,\Gamma_1} = \left|\bar\phi_0^* - \bar\phi_{h,0}^*\right|_{1,\Gamma_1} \le CT^2 \inf_{w\in V_h} \left|\bar\phi_0^* - w\right|_{1,\Gamma_1}. \tag{5.2}$$

If T is large enough, (5.1) can be regarded as a singularly perturbed problem, for which the best approximation given by a uniform mesh cannot reach the optimal convergence rate due to the existence of a boundary layer.

We now consider Problem II with a finite T^*. The minimizer $\bar\phi^*$ of $\hat S(\bar\phi)$ satisfies the weak form of (5.1):

$$\left\langle \left(\bar\phi^*\right)', v'\right\rangle_{\Gamma_1} = -\hat T^2\left(\bar\phi^*\right)\left\langle A\bar\phi^*, Av\right\rangle_{\Gamma_1} \quad \forall\, v \in H_0^1(\Gamma_1). \tag{5.3}$$

The minimizer $\bar\phi_h^*$ of $\hat S_h(\bar\phi_h)$ satisfies the discrete weak form:

$$\left\langle \left(\bar\phi_h^*\right)', v'\right\rangle_{\Gamma_1} = -\hat T^2\left(\bar\phi_h^*\right)\left\langle A\bar\phi_h^*, Av\right\rangle_{\Gamma_1} \quad \forall\, v \in V_h. \tag{5.4}$$

We have the following a priori error estimate for Problem II with a finite T^*.

PROPOSITION 5.1. *Consider a subsequence $\bar\phi_h^*$ converging weakly to $\bar\phi^*$ in $H^1(\Gamma_1)$ as $h \to 0$. Assume that $\bar\phi^*$ and $\bar\phi_h^*$ satisfy* (5.3) *and* (5.4), *respectively. For problem* II *with a finite T^*, there exists a constant $C \sim (T^*)^2$ such that*

$$\left|\bar\phi^* - \bar\phi_h^*\right|_{1,\Gamma_1} = \left|\bar\phi_0^* - \bar\phi_{h,0}^*\right|_{1,\Gamma_1} \le C \inf_{w\in V_h} \left|\bar\phi_0^* - w\right|_{1,\Gamma_1} \tag{5.5}$$

when h is small enough.

Proof. Let η be the best approximation of $\bar\phi^*$ on $V_h \oplus \phi_L$, i.e.,

$$\left|\bar\phi^* - \eta\right|_{1,\Gamma_1} = \inf_{w\in V_h\oplus\phi_L} \left|\bar\phi^* - w\right|_{1,\Gamma_1}.$$

We then have

$$\langle(\bar\phi^* - \eta)', w'\rangle = 0 \quad \forall\, w \in V_h,$$

where $\bar\phi^* - \eta \in H_0^1(\Gamma_1)$. Consider

$$\begin{aligned}
\left|\bar\phi_h^* - \eta\right|_{1,\Gamma_1}^2 &= \left\langle(\bar\phi_h^* - \bar\phi^*)', (\bar\phi_h^* - \eta)'\right\rangle_{\Gamma_1} + \left\langle(\bar\phi^* - \eta)', (\bar\phi_h^* - \eta)'\right\rangle_{\Gamma_1}\\
&= \left\langle(\bar\phi_h^* - \bar\phi^*)', (\bar\phi_h^* - \eta)'\right\rangle_{\Gamma_1}\\
&= -\left\langle(\hat T^2(\bar\phi_h^*)\bar\phi_h^* - \hat T^2(\bar\phi^*)\bar\phi^*), A^2(\bar\phi_h^* - \eta)\right\rangle_{\Gamma_1}\\
&= -\left\langle(\hat T^2(\bar\phi_h^*)\bar\phi_h^* - \hat T^2(\eta)\eta), A^2(\bar\phi_h^* - \eta)\right\rangle_{\Gamma_1}\\
&\quad -\left\langle(\hat T^2(\eta)\eta - \hat T^2(\bar\phi^*)\bar\phi^*), A^2(\bar\phi_h^* - \eta)\right\rangle_{\Gamma_1}\\
&= I_1 + I_2.
\end{aligned} \tag{5.6}$$

We look at I_2 first. Note that

$$\begin{aligned}
&|\hat{T}^2(\eta) - \hat{T}^2(\bar{\phi}^*)| \\
&= \left| \frac{|\eta|^2_{1,\Gamma_1}}{|A\eta|^2_{0,\Gamma_1}} - \frac{|\bar{\phi}^*|^2_{1,\Gamma_1}}{|A\bar{\phi}^*|^2_{0,\Gamma_1}} \right| \\
&= \left| \frac{|\eta|^2_{1,\Gamma_1} - |\bar{\phi}^*|^2_{1,\Gamma_1}}{|A\eta|^2_{0,\Gamma_1}} + \frac{|\bar{\phi}^*|^2_{1,\Gamma_1}(|A\bar{\phi}^*|^2_{0,\Gamma_1} - |A\eta|^2_{0,\Gamma_1})}{|A\eta|^2_{0,\Gamma_1}|A\bar{\phi}^*|^2_{0,\Gamma_1}} \right| \\
&\le C_{\hat{T}}(\eta, \bar{\phi}^*)|\eta - \bar{\phi}^*|_{1,\Gamma_1}, \qquad (5.7)
\end{aligned}$$

where

$$C_{\hat{T}}(\eta, \bar{\phi}^*) = \frac{|\eta|_{1,\Gamma_1} + |\bar{\phi}^*|_{1,\Gamma_1}}{|A\eta|^2_{0,\Gamma_1}} + \frac{|\bar{\phi}^*|^2_{1,\Gamma_1}(|A\eta|_{0,\Gamma_1} + |A\bar{\phi}^*|_{0,\Gamma_1})\|A\|C_p}{|A\eta|^2_{0,\Gamma_1}|A\bar{\phi}^*|^2_{0,\Gamma_1}}$$

and C_p is the Poincaré constant. Then we have

$$\begin{aligned}
|I_2| &= \left| \left\langle (\hat{T}^2(\eta)\eta - \hat{T}^2(\bar{\phi}^*)\bar{\phi}^*), A^2(\bar{\phi}^*_h - \eta) \right\rangle_{\Gamma_1} \right| \\
&\le \left| \left\langle \hat{T}^2(\eta)(\eta - \bar{\phi}^*), A^2(\bar{\phi}^*_h - \eta) \right\rangle_{\Gamma_1} \right| \\
&\quad + \left| \left\langle (\hat{T}^2(\eta) - \hat{T}^2(\bar{\phi}^*))\bar{\phi}^*, A^2(\bar{\phi}^*_h - \eta) \right\rangle_{\Gamma_1} \right| \\
&\le (\hat{T}^2(\eta)C_p^2\|A\|^2 + C_{\hat{T}}(\eta, \bar{\phi}^*)|A\bar{\phi}^*|_{0,\Gamma_1}\|A\|C_p)|\eta - \bar{\phi}^*|_{1,\Gamma_1}|\bar{\phi}^*_h - \eta|_{1,\Gamma_1} \\
&= C_{I_2}(\eta, \bar{\phi}^*)|\eta - \bar{\phi}^*|_{1,\Gamma_1}|\bar{\phi}^*_h - \eta|_{1,\Gamma_1}. \qquad (5.8)
\end{aligned}$$

By the definition of η, we have

$$\lim_{h\to 0}|\eta|_{1,\Gamma_1} = |\bar{\phi}^*|_{1,\Gamma_1}, \quad \lim_{h\to 0}|A\eta|_{0,\Gamma_1} = |A\bar{\phi}^*|_{0,\Gamma_1}.$$

We then have

$$\lim_{h\to 0} C_{I_2}(\eta, \bar{\phi}^*) = 2M + 3M^2,$$

where $M = \|A\|C_pT^*$.

We now look at I_1. Since $\lim_{h\to 0}\hat{T}(\bar{\phi}^*_h) = \lim_{h\to 0}\hat{T}(\eta) = T^*$ and $T^* < \infty$, we know that when h is small enough, $I_1 \sim -(T^*)^2 \left\langle (\bar{\phi}^*_h - \eta), A^2(\bar{\phi}^*_h - \eta) \right\rangle_{\Gamma_1} < 0$. Combining this fact with (5.6) and (5.8), we have that for h small enough there exists a constant $C > 2M + 3M^2$ such that

$$\left|\bar{\phi}^*_h - \eta\right|_{1,\Gamma_1} \le C\left|\bar{\phi}^* - \eta\right|_{1,\Gamma_1} = C \inf_{w\in V_h\oplus\phi_L} \left|\bar{\phi}^* - w\right|_{1,\Gamma_1}. \qquad \square$$

To this end, we obtain an a priori error estimate similar to that for Problem I with a fixed T. Since T^* can be arbitrarily large, we know that the optimal convergence rate may degenerate when a boundary layer exists. Using Proposition 5.1, we can easily obtain the optimal convergence rate with respect to the error of the action functional:

$$|\hat{S}(\bar{\phi}^*) - \hat{S}(\bar{\phi}^*_h)| \sim |\delta^2\hat{S}(\bar{\phi}^*)| \sim |\bar{\phi}^*_h - \bar{\phi}^*|^2_{1,\Gamma_1}, \qquad (5.9)$$

where the second-order variation can be obtained with respect to the perturbation function $\delta\bar{\phi} = \bar{\phi}^* - \bar{\phi}^*_h$.

The convergence rate for T^* is also optimal. For a general case, we have the first-order variation of $\hat{T}^2$ at $\bar{\phi}^*$ with a test function $\delta\bar{\phi}$ as

$$\begin{aligned}|\delta(\hat{T}^2)| &= \left|\frac{2\langle(\bar{\phi}^*)'', \delta\bar{\phi}\rangle_{\Gamma_1} + 2(T^*)^2\langle(\nabla b)^{\mathsf{T}} b, \delta\bar{\phi}\rangle_{\Gamma_1}}{|b(\bar{\phi}^*)|^2_{0,\Gamma_1}}\right| \\ &\leq 2|b(\bar{\phi}^*)|^{-2}_{0,\Gamma_1}\left(|\bar{\phi}^*|_{2,\Gamma_1} + (T^*)^2 K|b(\bar{\phi}^*)|_{0,\Gamma_1}\right)|\delta\phi|_{0,\Gamma_1}.\end{aligned}$$

Also note that the second-order variation has the same order as $|\delta\phi|^2_{1,\Gamma_1}$. Let $\delta\phi = \bar{\phi}^*_h - \bar{\phi}^*$. From Proposition 5.1, we know the second-order variation has an optimal convergence rate $|\bar{\phi}^*_h - \bar{\phi}^*|^2_{1,\Gamma_1} \sim O(h^2)$ when $\bar{\phi}^* \in H^2(\Gamma_1)$. If $|\bar{\phi}^*_h - \bar{\phi}^*|_{0,\Gamma_1}$ can also reach its optimal rate, which is of order $O(h^2)$, the overall convergence rate for T^* is of order $O(h^2)$. We will not analyze the optimal convergence of $\bar{\phi}^*_h$ in the L^2 norm here, but only provide numerical evidence of the optimal convergence rate for T^* in the next section.

6. Numerical experiments.

We will use the following simple linear stochastic ODE system to demonstrate our analysis results:

$$dX(t) = AX(t)\,dt + \sqrt{\varepsilon}\,dW(t), \tag{6.1}$$

where

$$A = B^{-1}JB = \begin{bmatrix} a & -b \\ b & a \end{bmatrix}\begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}\begin{bmatrix} a & b \\ -b & a \end{bmatrix},$$

with $a = 1/3$, $b = \sqrt{8}/3$, $\lambda_1 = -10$, and $\lambda_2 = -2$. Then $z = (0, 0)^{\mathsf{T}}$ is a stable fixed point. For the corresponding deterministic system, namely when $\varepsilon = 0$, and any given point $X(0) = x \neq z$ in the phase space, the trajectory $X(t) = e^{tA}x$ converges to z as $t \to \infty$. When noise exists, this trajectory is also the MAP ϕ^* from x to $e^{tA}x$ with $T^* = t$, since $V(x, e^{tA}x) = 0$. Moreover, if the ending point is z, then $T^* = \infty$. This obviously is not an exit problem, which is a typical application of MAM. However, it includes most of the numerical difficulties of MAM, and the trajectory can serve as an exact solution, which simplifies the discussions.

Consider the MAP from x ($\neq z$) to $e^{tA}x$ such that $T^* = t$. Since the MAP corresponds to a trajectory, we can use the value of the action functional as the measure of error with an optimal rate $O(h^2) \sim O(N^{-2})$ (see (5.9)), where N is the number of elements. We will look at the following two cases:

(i) T^* is finite and small. According to Theorem 4.5, $\bar{\phi}_h$ converges to $\bar{\phi}^*$. Since T^* is small, according to Proposition 5.1, we expect an optimal convergence rate of $\bar{\phi}_h$ as $h \to 0$.

(ii) $T^* = \infty$. We will compare the convergence behavior between tMAM and MAM with a fixed large T. According to Theorem 4.11, we have the convergence in $\bar{C}^z_x$. However, the convergence behavior of this case is similar to that for a finite but large T^*, where we expect a deteriorated convergence rate.

6.1. Case (i).

Let $x = (1, 1)$. We use $e^A x$ as the ending point such that $T^* = 1$. In Figure 1 we plot the convergence behavior of tMAM with uniform linear finite element discretization. It is seen that the optimal convergence rate is reached for both the action functional and T^* estimated by $\hat{T}(\bar{\phi}^*_h)$.

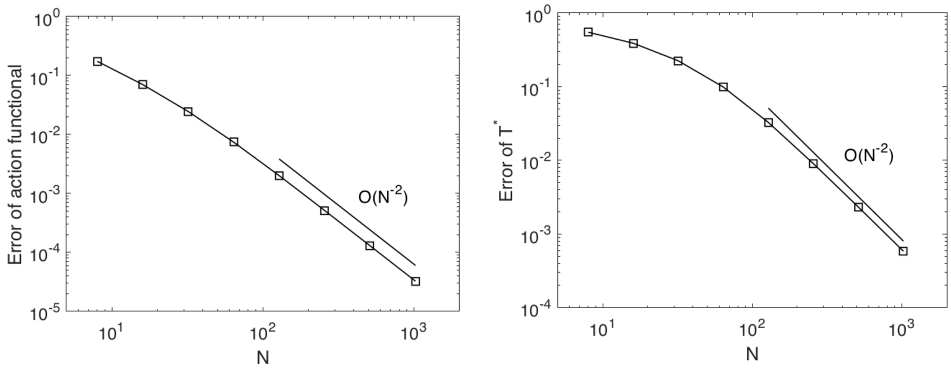

FIG. 1. *Convergence behavior of tMAM for Case* (i). *Left: Errors of the action functional. Right: Errors of* T^*.

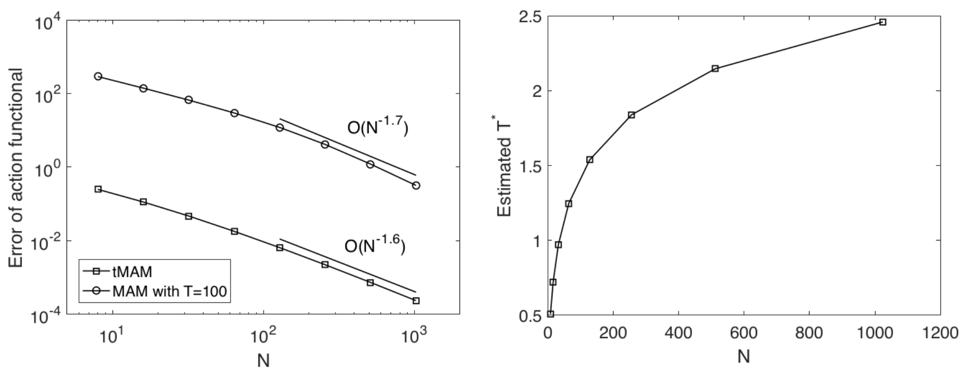

FIG. 2. *Convergence behavior of tMAM and MAM with a fixed* T *for Case* (ii). *Left: Errors of the action functional. Right: Estimated* T^* *of tMAM, i.e.,* $\hat{T}(\bar{\phi}_h^*)$.

6.2. Case (ii). For this case, we still use $x = (1, 1)$ as the starting point. The ending point is chosen as $a = (0, 0)^{\mathsf{T}}$ such that $T^* = \infty$. Besides tMAM, we use MAM with a fixed T to approximate this case, where T is supposed to be large. In general, we do not have a criterion to define how large T must be because the accuracy is affected by two competing issues: (1) $T^* = \infty$ favors a large T, but (2) a fixed discretization favors a small T. This implies that for any given h, an "optimal" finite T exists. For the purpose of demonstration, we choose $T = 100$, which is actually too large from an accuracy point of view. Let $\phi_T^*(t)$ be the approximate MAP given by MAM with a fixed T. We know that $\bar{\phi}_T^*(s) = \phi_T^*(t/T)$ yields a smaller action with the integration time $\hat{T}(\bar{\phi}_T^*(s))$. In this sense, no matter what T is chosen, for the same discretization tMAM will always provide a better approximation than MAM with a fixed T. The reason we use an overlarge T is to demonstrate the deterioration of the convergence rate. In Figure 2, we plot the convergence behavior of tMAM and MAM with $T = 100$ on the left, and the estimated T^* given by tMAM on the right. It is seen that the convergence is slower than $O(N^{-2})$, as we have analyzed in section 5. For the same discretization, tMAM has an accuracy that is several orders of magnitude better than MAM with $T = 100$. In the right plot of Figure 2, we see that

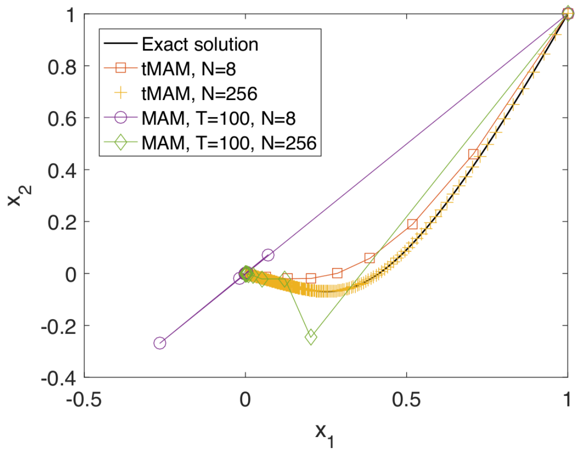

FIG. 3. *Approximate MAPs given by tMAM and MAM with a fixed T for Case* (ii).

the optimal integration time for a certain discretization is actually not large at all. This implies that MAM with a fixed T for Case (ii) is actually not very reliable. In Figure 3, we compare the MAPs given by tMAM and MAM with the exact solution $e^{tA}x$, where all symbols indicate the nodes of finite element discretization. First, we note that the number of effective nodes in MAM is small because of the scale separation of fast dynamics and small dynamics. Most nodes are clustered around the fixed point. This is called a problem of clustering (see [19, 26] for a discussion of this issue). Second, if the chosen T is too large, oscillation is observed in the paths given by MAM especially when the resolution is relatively low; on the other hand, tMAM does not suffer such an oscillation by adjusting the integration time according to the resolution. Third, although tMAM is able to provide a good approximation even with a coarse discretization, more than enough nodes are put into the region around the fixed point, which corresponds to the deterioration of the convergence rate. To recover the optimal convergence rate, we need to resort to adaptivity (see [22, 26] for the construction of the algorithm).

7. Summary. In this work, we have established some convergence results of minimum action methods based on linear finite element discretization. In particular, we have demonstrated that the minimum action method with optimal linear time scaling, i.e., tMAM, converges for Problem II whether the optimal integration time is finite or infinite.

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