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A HERMITE SPECTRAL METHOD FOR A FOKKER-PLANCK OPTIMAL CONTROL PROBLEM IN AN UNBOUNDED DOMAIN

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A Hermite spectral discretization method to approximate the solution of a Fokker-Planck optimal control problem in an unbounded domain is presented. It is proved that the solution of the corresponding discretized optimality system is spectrally accurate and the numerical scheme preserves the required conservativity property of the forward solution. The theoretical results are verified with numerical experiments.

KEY WORDS: *Fokker-Planck equation, optimal control theory, Hermite spectral discretization*

1. INTRODUCTION

The investigation of stochastic processes is a very active research field with many applications in technology, science, and finance. In particular, the possibility to control sequences of events subject to randomness is desirable for real applications. In this paper, we consider continuous-time stochastic processes described by the following multidimensional model:

$$\begin{cases} dX_t = b(X_t, t; u)\, dt + \sigma(X_t, t)\, dW_t \\ X_{t_0} = X_0, \end{cases} \tag{1}$$

where the state variable $X_t \in \mathbb{R}^d$ is subject to deterministic infinitesimal increments driven by the vector-valued drift function $b(x, t; u) \in \mathbb{R}^d$, and to random increments proportional to a multidimensional Wiener process $dW_t \in \mathbb{R}^m$, with stochastically independent components. The dispersion matrix $\sigma(x, t) \in \mathbb{R}^{d\times m}$ is full rank.

This is the so-called Itô stochastic differential equation (SDE) [7], where we model the action of a control function u with the purpose to drive the random process to attain desired objectives. In deterministic dynamics, the optimal control is achieved by finding the control law u that minimizes a given objective given by a cost functional $J(X, u)$ with the constraint given by a deterministic dynamical model. In the stochastic case, the state evolution X_t is random so that a direct insertion of a stochastic process into a deterministic cost functional will result in a random variable. To circumvent this difficulty and determine a robust control that does not depend on the single realizations of the process, an alternative approach was proposed in [1, 2], based on the fact that the state of a stochastic process can be completely characterized by the shape of its probability density function (PDF). The evolution of the PDF associated to the stochastic process X_t is modeled by the following Fokker-Planck (FP) model:

$$\partial_t f(x,t) - \frac{1}{2} \sum_{i,j=1}^{d} \partial^2_{x_i x_j} \left(a_{ij}(x,t)\, f(x,t)\right) + \sum_{i=1}^{d} \partial_{x_i} \left(b_i(x,t;u)\, f(x,t)\right) = 0, \tag{2}$$

$$f(x, t_0) = \rho(x), \tag{3}$$

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where f denotes the PDF function, and the diffusion coefficient is given by the positive-definite symmetric matrix $a = \sigma\,\sigma^\top/2$, with elements

$$a_{ij} = \frac{1}{2}\sum_{k=1}^{m} \sigma_{ik}\,\sigma_{jk}.$$

The initial PDF distribution ρ must be non-negative and normalized, $\int_\Omega \rho(x)dx = 1$. The FP model (2) is a parabolic problem on a multidimensional space domain, where the dimension corresponds to the number of components of the stochastic process; see also [19, 20]. Moreover, the problem (2)–(3) differs from a classical parabolic problem because of the additional requirements of positivity of solution and conservativeness. In fact, the FP equation with the given ρ guarantees the following:

$$f(x,t) \geq 0, \qquad \int_\Omega f(x,t)dx = 1, \qquad \text{for all } t \geq t_0.$$

The latter property results from the fact that we can write the FP equation in flux form, and vanishing fluxes on the boundary or at infinity are assumed. Notice that, in most cases, the FP problem is defined in an unbounded set in $\mathbb{R}^d$, because no bounds on the values of the state X_t are assumed. In this case, existence and uniqueness to the FP problem often rely on the concept of uniform parabolicity [8]; see, in particular, [2–4] and [14] and the references therein.

Our purpose is to investigate the discretization of the optimality system resulting from the optimal control strategy of [2] with a FP model in an unbounded domain. In this case, finite-difference or finite-element methods cannot be applied. By employing a suitable set of basis functions, spectral methods allow to treat unbounded domains. Since in our FP model, the solutions at infinity decay exponentially, we consider Hermite functions as basis functions, which are Hermite polynomials multiplied by a Gaussian. With this choice, we also take advantage of reducing the optimality system of partial differential equations (PDEs) into a system of ordinary differential equations (ODEs) with resulting sparse-band matrices of coefficients; see also [9, 10].

This paper is organized as follows. In Section 2, we discuss the FP equation in an unbounded domain. In Section 3, a FP control problem is formulated and the corresponding optimality system in an unbounded domain consisting of state, adjoint, and optimality condition equations is presented. The required properties and equipment for Hermite approximation are discussed in the Appendix. In Section 4, the Hermite spectral discretization of the state and adjoint equations is investigated. As a result of this section, the systems of PDEs, describing the state and the adjoint equations, are transformed to systems of ODEs. The matrix representation of these systems are presented, which provides an appropriate means to solve the system and to analyze the discretized scheme. In Section 5, the discretized scheme is analyzed, and the accuracy of the Hermite-spectral method is proved by showing that the error decreases spectrally as the number of expansion terms increases. We also investigate the conservativity of the scheme. The accuracy of the discretization method is investigated in Section 6 with numerical experiments. Section 7 presents a conclusion of this work.

2. THE FOKKER-PLANCK EQUATION IN AN UNBOUNDED DOMAIN

Denote with $f(x,t)$ the probability density to find the process X_t at $x = (x_1, \ldots, x_d) \in \Omega = \mathbb{R}^d$ at time t. Further, let $\hat{f}(x,t;y,s)$ denote the transition density probability distribution function for the stochastic Markov process to move from $y \in \Omega$ at time s to $x \in \Omega$ at time $t \geq s$, that is related to the probability of the process $X(t) \in (x, x+dx)$ conditioned to $X(s) = y$. We have

$$\hat{f}(x,t;y,s)dx = \wp\{X(t) \in (x, x+dx) | X(s) = y\},$$

where $\wp$ is a measure on probability space. Both $f(x,t)$ and $\hat{f}(x,t;y,s)$ are nonnegative functions and the following holds:

$$\hat{f}(x,t;y,s) \geq 0, \qquad \int_\Omega \hat{f}(x,t;y,s)\,dx = 1 \quad \text{for all } t \geq s. \tag{4}$$

That is, the transition probability density should be non-negative for all values of the arguments and be normalized to one after integration over the destination state.

If $\rho(y,s)$ is the given initial density probability of the process at time s, then we have that the probability density of the process at time $t > s$ is given by the following:

$$f(x,t) = \int_\Omega \hat{f}(x,t;y,s)\rho(y,s)\,dy. \tag{5}$$

Also ρ must be non-negative and normalized $\int_\Omega \rho(y,s)dy = 1$.

In our discussion, the Fokker-Planck equation is defined on $Q = \Omega \times (0,T)$, and we consider an unbounded domain, $\Omega = \mathbb{R}^d$. We assume that the initial distribution ρ is given (we drop s in the initial distribution) and hence the Fokker-Planck equation modeling the evolution of the probability density f satisfying (4) at all times is given by (2)–(3).

Next, we introduce some assumptions on the FP model that guarantee its solvability. We have the following:

Assumption 1.

1. *The coefficient function a_{ij} is bounded and satisfies the following uniform ellipticity condition for a constant $\theta > 0$:*
$$\sum_{ij=1}^d a_{ij}(x,t)\xi_i\xi_j \geq \theta\,|\xi|^2, \qquad \forall\, \xi \in \mathbb{R}^d,\ (x,t) \in Q.$$
2. *The coefficient functions b_i and $\partial_{x_i} a_{ij}$, $i,j = 1,\ldots,d$, satisfy the following:*
$$b_i,\ \partial_{x_i} a_{ij} \in L^q(0,T;L^p(\Omega))$$
where p and q are such that $2 < p, q \leq \infty$, and $d/2p + 1/q < 1/2$.
3. *The functions $\partial_{x_i} b_i$, $i = 1,\ldots,d$, satisfy*
$$\partial_{x_i} b_i \in L^q(0,T;L^p(\Omega))$$
where p and q are such that $1 < p, q \leq \infty$, and $d/2p + 1/q < 1$.

These assumptions were introduced in [3] to prove existence and uniqueness of non-negative solutions of parabolic problems. In [2], the results of [3] have been specialized to prove existence, uniqueness, and positivity of solutions to the forward FP problem (2)–(3) in a bounded domain. We have the following:

Theorem 1. *Suppose that b_i and a_{ij} in (2) satisfy the Assumption 1, and take the initial condition $\rho \in H_0^1(\Omega)$ and homogeneous boundary conditions on $\Sigma = \partial\Omega \times (0,T)$. Then there exists a unique weak solution f to (2)–(3). Further, the solution f has the following additional property:*

If $0 \leq \rho \leq m$ a.e. in Ω, then
$$0 \leq f(x,t) \leq m(1 + C\,k), \qquad \text{in } Q$$
where $k = 1/2\sum_{i=1}^d \|\sum_{j=1}^d \partial_{x_j} a_{ij}\|_{p,q} + \|\sum_{i=1}^d \partial_{x_i} b_i\|_{p,q}$ and C depends only on T, Ω, and the structure of the FP operator.

We use this theorem to discuss existence, uniqueness, and positivity of the solution to the FP problem (2)–(3) in an unbounded domain $\Omega = \mathbb{R}^d$. To this end, we define some special boundary value problems, as is proposed in [3].

Let $\Omega^k = \{x; |x| < k\}$ and $Q^k = \Omega^k \times (0,T)$. For each integer $k \geq 3$, let $\zeta^k = \zeta^k(x)$ denote a $C_0^\infty(\mathbb{R}^n)$ function such that $\zeta^k = 1$ for $|x| \leq k-2$, $\zeta^k = 0$ for $|x| \geq k-1$, $0 \geq \zeta^k \leq 1$ and $|\partial_x \zeta^k|$ is bounded independent of k. According to Theorem 1, for each k there exists a unique and bounded weak solution f^k to the boundary value problem

$$\begin{aligned} \partial_t f^k - \frac{1}{2}\sum_{i,j=1}^d \partial^2_{x_i x_j}\left(a_{ij}\,f^k\right) + \sum_{i=1}^d \partial_{x_i}\left(b_i(u)\,f^k\right) = 0 \quad &\text{in } Q^k, \\ f^k(x,0) = \zeta^k(x)\rho(x) \quad &\text{in } \Omega^k, \end{aligned} \tag{6}$$

with homogeneous boundary conditions. Extend the domain of definition of f^k by setting $f^k = 0$ for $|x| \geq k$.

In [3] one can find the arguments which prove the following theorem.

Theorem 2. *If b_i and a_{ij} in (2) satisfy the Assumption 1, the function f^k in (6) is bounded, $\rho \in H^1(\Omega)$, and $\rho \geq 0$ almost everywhere in Ω, then the problem (2)–(3) possesses a unique and non-negative weak solution.*

Although the results presented in [3] and later generalized in [12] prove the existence of a unique non-negative solution for our problem belonging to the space $L^\infty((0,T); L^2_{loc}(\Omega)) \cap L^2((0,T); H^1_{loc}(\Omega))$, the arguments provided in [13] show that this solution may have higher regularity. In fact, we have that for $r > 0$, $f \in H^{r+2,r/2+1}(Q)$ as long as $\rho \in H^{r+2}(\Omega)$ and the coefficients a_{ij} and b_i belong to $H^{r,r/2}(Q)$.

Notice that in our case and in many applications the FP parameter functions are smooth and Assumption 1 and the assumptions in [13] are immediately satisfied. For additional results on the Fokker-Planck equation with irregular coefficients see [14].

3. A FOKKER-PLANCK OPTIMAL CONTROL PROBLEM

The control strategy proposed in [2] requires to minimize an objective under the constraint given by the FP equation. The implementation of this strategy is an instance of the class of model predictive control (MPC) schemes [11], which is widely used in engineering applications to design closed-loop algorithms. To illustrate this method, let $(0, T)$ be the time interval where the process is considered. In [2], the time interval is subdivided in time windows of size Δt and on each of these windows an open-loop FP optimal control problem is solved that uses the solution PDF of the previous time window as initial condition, and the target is specified at the end of each window. This procedure is repeated by receding the time horizon until the last time window is reached. In particular, the approach in [2] considers vector-valued constant control functions on each time window such that along the interval $(0, T)$ a piecewise constant control is obtained. For the reason of clarity in error analysis, we focus on one time window, that we identify with $(0, T)$.

Now, within this framework, we formulate the problem to determine a control $u \in \mathbb{R}^\ell$ such that starting with an initial distribution ρ the process evolves towards a desired target probability density $f_d(x, t)$ at time $t = T$. This objective can be formulated by the following tracking functional:

$$J(f, u) := \frac{1}{2}\|f(\cdot, T) - f_d(\cdot, T)\|^2_{w_\alpha} + \frac{\nu}{2}|u|^2, \tag{7}$$

where $|u|^2 = u_1^2 + \ldots + u_\ell^2$, and $\nu > 0$ is a constant. With $\|\cdot\|^2_{w_\alpha}$ we denote the following:

$$\|v\|^2_{w_\alpha} = \int_\Omega v(x)^2 w_\alpha(x) dx$$

where $w_\alpha(x) = \exp(\alpha^2 x^2)$ is a weight function, and $\alpha > 0$ must be appropriately chosen.

The optimal control problem to find u that minimizes the objective J subject to the constraint given by the FP equation is formulated by the following:

$$\min \frac{1}{2}\|f(\cdot, T) - f_d(\cdot, T)\|^2_{w_\alpha} + \frac{\nu}{2}|u|^2 \tag{8}$$

$$\partial_t f(x,t) - \frac{1}{2}\sum_{i,j=1}^{d} \partial^2_{x_i x_j}\left(a_{ij}(x,t)\, f(x,t)\right) + \sum_{i=1}^{d} \partial_{x_i}\left(b_i(x,t;u)\, f(x,t)\right) = 0 \tag{9}$$

$$f(x, 0) = \rho(x). \tag{10}$$

Notice that for a given control function u, Theorem 2 states that the solution of the FP model (9)–(10) is uniquely determined. We denote this dependence by $f = f(u)$ and one can prove that the mapping $u \to f(u)$ is twice differentiable [16]. Therefore, we can introduce the so-called reduced cost functional $\hat{J}$ given by

$$\hat{J}(u) = J(f(u), u). \tag{11}$$

Correspondingly, a local minimum u^* of $\hat{J}$ is characterized by $\hat{J}'(u^*; \delta u) = 0$ for all $\delta u \in \mathbb{R}^\ell$.

To characterize the solution to our optimization problem, we consider the Lagrange formalism and formulate the first-order optimality conditions. Consider the Lagrange functional

$$\begin{aligned} L(f,u,p) &= J(f,u) \\ &+ \int_\Omega \int_0^T \left(\partial_t f - \frac{1}{2} \sum_{i,j=1}^{d} \partial^2_{x_i x_j} \left(a_{ij}\, f \right) + \sum_{i=1}^{d} \partial_{x_i} \left(b_i(u)\, f \right) \right) p\, w_\alpha \, dx\, dt, \end{aligned}$$

where $p = p(x,t)$ represents the Lagrange multiplier. The first-order optimality conditions for our FP optimal control problem are formally derived by equating to zero the Fréchet derivatives of the Lagrange function with respect to the set of variables (f,u,p); see, e.g., [5, 16]. The optimality conditions result in the following optimality system. We have

$$\begin{aligned} \partial_t f - \frac{1}{2} \sum_{i,j=1}^{d} \partial^2_{x_i x_j} \left(a_{ij}\, f \right) + \sum_{i=1}^{d} \partial_{x_i} \left(b_i(u)\, f \right) = 0 \quad &\text{in } Q, \quad \text{(state equation)} \\ f(x,0) = \rho(x) \quad &\text{in } \Omega, \quad \text{(initial condition)} \\ -\partial_t (p w_\alpha) - \frac{1}{2} \sum_{i,j=1}^{d} a_{ij}\, \partial^2_{x_i x_j} \left(p w_\alpha \right) - \sum_{i=1}^{d} b_i(u)\, \partial_{x_i} \left(p w_\alpha \right) = 0 \quad &\text{in } Q, \quad \text{(adjoint equation)} \\ -p(x,T) = f(x,T) - f_d(x,T) \quad &\text{in } \Omega, \quad \text{(terminal condition)} \\ \nu\, u_l + \left\langle \sum_{i=1}^{d} \partial_{x_i} \left(\frac{\partial b_i}{\partial u_l}\, f \right), p \right\rangle_{w_\alpha} = 0 \quad \text{in } Q, \quad l = 1, \ldots, \ell \quad &\text{(optimality equations)} \end{aligned} \tag{12}$$

where we use the following inner product:

$$\langle \phi, \psi \rangle_{w_\alpha} = \int_0^T \int_\Omega \phi(x,t)\, \psi(x,t)\, w_\alpha(x)\, dx\, dt.$$

Notice that the state variable evolves forward in time and the adjoint variable evolves backwards in time. We remark that the FP equation is a particular instance of the forward Kolmogorov equation and the adjoint equation resembles the backward Kolmogorov equation.

It should appear [1, 2] clearly that the lth component of the reduced gradient $\nabla \hat{J}$ is given by

$$(\nabla \hat{J})_l = \nu\, u_l + \left\langle \sum_{i=1}^{d} \partial_{x_i} \left(\frac{\partial b_i}{\partial u_l}\, f \right), p \right\rangle_{w_\alpha}, \qquad l = 1, \ldots, \ell, \tag{13}$$

where $p = p(u)$ is the solution of the adjoint equation for the given $f(u)$.

Notice that the optimization problem given by (8)–(10) represents a bilinear control problem where the dependence of the state f on the control u is nonlinear and the corresponding optimization problem is nonconvex. However, standard arguments [1, 2, 5, 16, 21] allow to prove existence of optimal solutions of the open-loop control in $(0,T)$.

4. HERMITE DISCRETIZATION OF THE FP OPTIMALITY SYSTEM

We consider a FP control problem corresponding to a representative stochastic process given by the Ornstein-Uhlenbeck process, and for simplicity we focus on a one-dimensional setting, $d = 1$, in which the function b is linear and a is constant. We have $b(x,t;u) = \gamma x + u$ and $a(x,t) = 2c$, where $\gamma < 0$, u and $c > 0$ are constants. In this case, the optimality system is given by

$$
\begin{aligned}
\partial_t f(x,t) - c\partial_{xx} f(x,t) + \partial_x\left((\gamma x + u) f(x,t)\right) = 0, \quad & \text{in } Q,\\
f(x,0) = \rho(x), \quad & \text{in } \Omega,\\
-\partial_t (p(x,t) w_\alpha(x)) - c\partial_{xx}(p(x,t) w_\alpha(x)) - (\gamma x + u)\partial_x (p(x,t) w_\alpha(x)) = 0, \quad & \text{in } Q,\\
-p(x,T) = f(x,T) - f_d(x,T), \quad & \text{in } \Omega,\\
\nu u + \langle \partial_x f(x,t), p(x,t)\rangle_{w_\alpha} = 0, \quad & \text{in } Q.
\end{aligned}
$$

For the analysis of the discretization of the optimality system with Hermite functions, we need to discuss some properties of the Hermite approximation space. For this purpose, we refer to the Appendix.

The state and adjoint variables are approximated in the space of Hermite functions as follows:

$$
f(x,t) = \sum_{n=0}^{\infty} \hat{f}_n(t)\tilde{\mathrm{H}}_n(x), \qquad p(x,t) = \sum_{n=0}^{\infty} \hat{p}_n(t)\tilde{\mathrm{H}}_n(x).
$$

For the adjoint equation, we note that the approximation

$$
p(x,t) = \sum_{n=0}^{\infty} \hat{p}_n(t)\tilde{\mathrm{H}}_n(x)
$$

is equivalent to

$$
p(x,t) w_\alpha(x) = \sum_{n=0}^{\infty} \frac{1}{\sqrt{2^n n!}} \hat{p}_n(t) H_n(\alpha x).
$$

The initial data $f(x,0) = \rho$ are also represented in the Hermite functions space by $\rho(x) = \sum_{n=0}^{\infty} \hat{f}_n^0 \tilde{\mathrm{H}}_n(x)$, where

$$
\hat{f}_n^0 = \frac{\alpha}{\sqrt{\pi}} \int_{\mathbb{R}} \rho(x)\tilde{\mathrm{H}}_n(x) w_\alpha(x)dx, \quad n \geq 0.
$$

Since $p(x,T) = f_d(x,T) - f(x,T)$, after calculating the numerical solution of the forward equation, the terminal condition for the adjoint variable p can be approximated by $p(x,T) = \sum_{n=0}^{\infty} \hat{p}_{T,n}\tilde{\mathrm{H}}_n(x)$, where

$$
\hat{p}_{T,n} = \frac{\alpha}{\sqrt{\pi}} \int_{\mathbb{R}} f_d(x,T)\tilde{\mathrm{H}}_n(x) w_\alpha(x)dx - \hat{f}_n, \quad n \geq 0.
$$

Introducing the Hermite expansions for f and p into the state and adjoint equations, for $n \geq 0$ we have

$$
\frac{d}{dt}\hat{f}_n(t) = n\gamma \hat{f}_n(t) + \alpha u\sqrt{2n}\hat{f}_{n-1}(t) + (\gamma + 2\alpha^2 c)\sqrt{n(n-1)}\hat{f}_{n-2}(t), \tag{14}
$$

with $\hat{f}_{-1} = 0$, $\hat{f}_{-2} = 0$, and

$$
-\frac{d}{dt}\hat{p}_n(t) = n\gamma \hat{p}_n(t) + \alpha u\sqrt{2(n+1)}\hat{p}_{n+1}(t) + (\gamma + 2\alpha^2 c)\sqrt{(n+2)(n+1)}\hat{p}_{n+2}(t). \tag{15}
$$

The Eqs. (14)–(15) represent two infinite systems of ODEs. These systems are truncated by considering the approximations

$$
[\hat{f}_{\Delta,0}(t), \hat{f}_{\Delta,1}(t), \cdots, \hat{f}_{\Delta,N}(t)] \approx [\hat{f}_0(t), \hat{f}_1(t), \cdots],
$$

and

$$
[\hat{p}_{\Delta,0}(t), \hat{p}_{\Delta,1}(t), \cdots, \hat{p}_{\Delta,N}(t)] \approx [\hat{p}_0(t), \hat{p}_1(t), \cdots].
$$

Therefore, the systems of ODEs which we solve are as follows:

$$
\begin{aligned}
\frac{d}{dt}\hat{f}_{\Delta,n}(t) = n\gamma \hat{f}_{\Delta,n}(t) + \alpha u\sqrt{2n}\hat{f}_{\Delta,n-1}(t) + (\gamma + 2\alpha^2 c)\sqrt{n(n-1)}\hat{f}_{\Delta,n-2}(t),\\
\hat{f}_{\Delta,n}(0) = \hat{\rho}_n,
\end{aligned} \tag{16}
$$

and

$$-\frac{d}{dt}\hat{p}_{\Delta,n}(t) = n\gamma\hat{p}_{\Delta,n}(t) + \alpha u\sqrt{2(n+1)}\hat{p}_{\Delta,n+1}(t) + (\gamma+2\alpha^2 c)\sqrt{(n+2)(n+1)}\hat{p}_{\Delta,n+2}(t), \quad \hat{p}_{\Delta,n}(T) = \hat{p}_{T,n}, \tag{17}$$

for $0 \le n \le N, 0 \le t \le T$, with $\hat{f}_{\Delta,i} = 0$ and $\hat{p}_{\Delta,N-i} = 0$, $i = -1, -2$. This corresponds to a Galerkin projection of $f(\cdot,t)$ and $p(\cdot,t)$ onto the Hermite approximation space

$$V_N = \text{span}\{\tilde{\text{H}}_n(x),\ 0 \le n \le N\}.$$

Defining $\tau = T - t$ and $\hat{q}_n(t) = \hat{p}_n(\tau)$, the last equation is equivalent to

$$\frac{d}{dt}\hat{q}_{\Delta,n}(t) = n\gamma\hat{q}_{\Delta,n}(t) + \alpha u\sqrt{2(n+1)}\hat{q}_{\Delta,n+1}(t) + (\gamma+2\alpha^2 c)\sqrt{(n+2)(n+1)}\hat{q}_{\Delta,n+2}(t), \quad \hat{q}_{\Delta,n}(0) = \hat{p}_{T^k,n}. \tag{18}$$

The systems (16) and (18) can be written in the following matrix form:

$$\frac{d\hat{f}_\Delta}{dt} = M_f \hat{f}_\Delta, \tag{19}$$

and

$$\frac{d\hat{q}_\Delta}{dt} = M_q \hat{q}_\Delta, \tag{20}$$

where

$$\hat{f}_\Delta = [\hat{f}_{\Delta,0}(t), \hat{f}_{\Delta,1}(t), \cdots, \hat{f}_{\Delta,N}(t)]^T,$$
$$\hat{q}_\Delta = [\hat{q}_{\Delta,0}(t), \hat{q}_{\Delta,1}(t), \cdots, \hat{q}_{\Delta,N}(t)]^T,$$

and M_f and M_q are two $(N+1)\times(N+1)$ three-diagonal matrices with the elements

$$(M_f)_{ij} = \begin{cases} n\gamma, & i=j, \\ \alpha u\sqrt{2n}, & i-j=1, \\ (\gamma+2\alpha^2 c)\sqrt{n(n-1)}, & i-j=2, \\ 0, & \text{otherwise}, \end{cases} \qquad 1 \le i,j \le N+1,$$

$$(M_q)_{ij} = \begin{cases} n\gamma, & j=i, \\ \alpha u\sqrt{2(n+1)}, & j-i=1, \\ (\gamma+2\alpha^2 c)\sqrt{(n+2)(n+1)}, & j-i=2, \\ 0, & \text{otherwise}, \end{cases} \qquad 1 \le i,j \le N+1,$$

where $n = i-1$. Notice that the first row in M_f and also the first column in M_q are zero.

Once we have calculated $\hat{f}_\Delta$ and $\hat{q}_\Delta$ by

$$\hat{f}_\Delta(t) = \exp(M_f t)\,\hat{f}^0_\Delta, \quad \text{and} \quad \hat{q}_\Delta(t) = \exp(M_q t)\,\hat{q}^0_\Delta,$$

the optimality variable u can be computed. Representing the approximated solutions by

$$f_\Delta(x,t) = \sum_{n=0}^{N} \hat{f}_{\Delta,n}(t)\tilde{\text{H}}_n(x), \quad \text{and} \quad p_\Delta(x,t) = \sum_{n=0}^{N} \hat{p}_{\Delta,n}(t)\tilde{\text{H}}_n(x),$$

we have

$$\begin{aligned}\int_{\mathbb{R}}(\partial_x f_\Delta)p_\Delta w_\alpha dx &= \int_{\mathbb{R}}\left(\sum_{n=0}^{N}\hat{f}_{\Delta,n}\frac{d}{dx}\tilde{\mathrm{H}}_n(x)\right)\left(\sum_{n=0}^{N}\hat{p}_{\Delta,n}\tilde{\mathrm{H}}_n(x)\right)w_\alpha dx\\ &= -\alpha\int_{\mathbb{R}}\left(\sum_{n=0}^{N}\sqrt{2(n+1)}\hat{f}_{\Delta,n}\tilde{\mathrm{H}}_{n+1}(x)\right)\left(\sum_{n=0}^{N}\hat{p}_{\Delta,n}\tilde{\mathrm{H}}_n(x)\right)w_\alpha dx\\ &= -\alpha\sum_{n=0}^{N}\sum_{k=0}^{N}\sqrt{2(n+1)}\hat{f}_{\Delta,n}\hat{p}_{\Delta,k}\int_{\mathbb{R}}\tilde{\mathrm{H}}_{n+1}(x)\tilde{\mathrm{H}}_k(x)w_\alpha dx\\ &= -\alpha\sum_{n=0}^{N-1}\sqrt{2(n+1)}\hat{f}_{\Delta,n}\hat{p}_{\Delta,n+1}\frac{\sqrt{\pi}}{\alpha}\\ &= -\sum_{n=0}^{N-1}\sqrt{2\pi(n+1)}\hat{f}_{\Delta,n}\hat{p}_{\Delta,n+1}.\end{aligned}$$

Then $\nu u + \langle\partial_x f(x,t), p(x,t)\rangle_{w_\alpha} = 0$ gives the following:

$$\begin{aligned}u_\Delta &= -\frac{1}{\nu}\langle\partial_x f_\Delta, p_\Delta\rangle_{w_\alpha} = -\frac{1}{\nu}\int_0^T\int_{\mathbb{R}}(\partial_x f_\Delta)p_\Delta w_\alpha dx\,dt\\ &= \frac{1}{\nu}\sum_{n=0}^{N-1}\sqrt{2\pi(n+1)}\int_0^T\hat{f}_{\Delta,n}\hat{p}_{\Delta,n+1}\,dt.\end{aligned}$$

5. ERROR ANALYSIS AND CONSERVATIVENESS OF THE HERMITE SPECTRAL DISCRETIZATION

We recall that substituting the Hermite expansion into the FP control system results in two infinite systems of linear ODEs. Corresponding to each system, there is a matrix M_∞, which is lower triangular for the state equation and upper triangular for the adjoint equation. To have a practical scheme, we have to truncate these matrices, or equivalently, consider some truncated systems of ODEs, which is a source of error in our discretization scheme. In the following, we investigate the influence of this error on the accuracy of our approximation method. Let $\|.\|_2$ be the Euclidean norm in $\mathbb{R}^{N+1}$.

Lemma 1. *Assuming N is sufficiently large so that there is no error in the spectral representation of the initial data, and $f(\cdot,t), f_d(\cdot,T) \in V_N$ for any $t\in[0,T]$, then*

$$\|\hat{f}_N - \hat{f}_\Delta\|_2 = 0, \qquad \textit{and} \qquad \|\hat{p}_N - \hat{p}_\Delta\|_2 = 0.$$

That is, there will be no error for the truncation of the infinite ODE systems.

Proof. For the forward case, no truncation error appears in calculating the Hermite coefficients $\hat{f}_n$ by solving the finite ODE system (19). This is because of the fact that the system (14) is uncoupled in the sense that for $m > n$ the value of $\hat{f}_n$ is independent of the value of $\hat{f}_m$. That is, $P_N f(\cdot,t) = f_\Delta(\cdot,t)$ for every $t\in[0,T]$.

The backward case can be analyzed following the procedure proposed in [6]. Consider M_∞ as the representing matrix for the ODE system transformed of the adjoint equation, and M the corresponding truncated matrix. The matrix M is obtained from M_∞ by removing all rows and columns with index larger than $N+1$. We can write

$$\hat{q} = e^{M_\infty t}\hat{q}^0 = \left(\sum_{j=0}^{\infty}\frac{t^j M_\infty^j}{j!}\right)\hat{q}^0 = \sum_{j=0}^{\infty}\frac{t^j}{j!}(M_\infty^j\hat{q}^0).$$

That is, for $n\geq 1$ we have

$$\hat{q}_{n-1} = \sum_{j=0}^{\infty}\frac{t^j}{j!}(M_\infty^j\hat{q}^0)_n = \sum_{j=0}^{\infty}\frac{t^j}{j!}b_n^j,$$

in which $b_n^j = (M_\infty^j \hat{q^0})_n$. Since we have assumed that $f(\cdot,t), f_d(\cdot,T) \in V_N$, we have $(\hat{q^0})_n = 0$ for $n > N+1$. Noting that M is an upper triangular matrix, it follows that $(M_\infty \hat{q^0})_n = 0$ for $n > N+1$. Therefore, for $j \geq 1$,

$$b_n^j = \sum_{k=1}^{N+1} (M_\infty^j)_{nk} (\hat{q^0})_k = \sum_{k=1}^{N+1} (M_\infty)_{nk} (M_\infty^{j-1} \hat{q^0})_k = \sum_{k=1}^{N+1} (M_\infty)_{nk} b_k^{j-1}.$$

Similarly $\hat{f}_{\Delta,n-1} = \sum_{j=0}^\infty (t^j/j!) b_{\Delta,n}^j$, with

$$b_{\Delta,n}^j = (M^j \hat{f_\Delta^0})_n = \begin{cases} \sum_{k=1}^{N+1} (M)_{nk} b_{\Delta,k}^{j-1}, & j \geq 1, n \leq N+1, \\ (\hat{f_\Delta^0})_n, & j=0, n \leq N+1, \\ 0, & n > N+1. \end{cases}$$

Therefore we have

$$\hat{f}_{n-1} - \hat{f}_{\Delta,n-1} = \sum_{j=0}^\infty \frac{t^j}{j!} (b_n^j - b_{\Delta,n}^j), \qquad n = 1, 2, \cdots, N+1,$$

and consequently by introducing $\theta_j = \sum_{n=1}^{N+1} |b_n^j - b_{\Delta,n}^j|$,

$$\sum_{n=1}^{N+1} |\hat{f}_{n-1} - \hat{f}_{\Delta,n-1}| \leq \sum_{j=0}^\infty \frac{t^j}{j!} \sum_{n=1}^{N+1} |b_n^j - b_{\Delta,n}^j| = \sum_{j=0}^\infty \frac{t^j}{j!} \theta_j.$$

Through the following argument, we find an upper bound for θ_j.

$$\theta_j = \sum_{n=1}^{N+1} |b_n^j - b_{\Delta,n}^j| + \sum_{n=1}^{N+1} \left| \sum_{k=1}^{N+1} (M_\infty)_{nk} b_k^{j-1} - \sum_{k=1}^{N+1} (M)_{nk} b_{\Delta,k}^{j-1} \right| = \sum_{n=1}^{N+1} \sum_{k=1}^{N+1} |(M)_{nk}| |b_k^{j-1} - b_{\Delta,k}^{j-1}|.$$

Therefore, we have

$$\theta_j \leq \sum_{k=1}^{N+1} |b_k^{j-1} - b_{\Delta,k}^{j-1}| \sum_{n=1}^{N+1} |(M)_{nk}| \leq cN^2 \sum_{k=1}^{N+1} |b_k^{j-1} - b_{\Delta,k}^{j-1}| = cN^2 \theta_{j-1},$$

for some positive constant c. With some calculations, we see that $\theta_j \leq (cN^2)^j \theta_0$. Since $b_n^0 = \hat{f}_n^0$ and $b_{\Delta,n}^0 = \hat{f_{\Delta,n}^0}$, $\theta_0 = \sum_{n=1}^{N+1} |b_n^0 - b_{\Delta,n}^0| = \sum_{n=0}^N |\hat{f}_n^0 - \hat{f_{\Delta,n}^0}|$ is the error in the representation of the initial data which is assumed to be zero. Therefore, we have

$$\|\hat{q}_N - \hat{q}_\Delta\|_2^2 = \sum_{n=0}^N |\hat{q}_n - \hat{q}_{\Delta,n}|^2 \leq \left(\sum_{n=0}^N |\hat{q}_n - \hat{q}_{\Delta,n}| \right)^2 = \left(\sum_{j=0}^\infty \frac{t^j}{j!} \theta_j \right)^2 \leq \left(\sum_{j=0}^\infty \frac{t^j}{j!} (cN^2)^j \theta_0 \right)^2 = 0,$$

and thence the desired result. □

To analyze the accuracy of the scheme, we first show that the approximations for the state and adjoint variables are spectrally convergent.

Theorem 3. *If $f, p \in L^\infty(0,T; H_{w_\alpha}^r(\mathbb{R}))$, $r > 1$, then for all $t \in [0,T]$ the following holds*

$$\|f(\cdot,t) - f_\Delta(\cdot,t)\|_{w_\alpha}^2 = O(N^{-r}), \quad \text{and} \quad \|p(\cdot,t) - p_\Delta(\cdot,t)\|_{w_\alpha}^2 = O(N^{-r}).$$

Proof. The argument is the same for f and p, so we only discuss the statement for f. We have

$$f(x,t) - f_\Delta(x,t) = \sum_{n=0}^{\infty} \hat{f}_n(t)\tilde{\mathrm{H}}_n(x) - \sum_{n=0}^{N} \hat{f}_{\Delta,n}(t)\tilde{\mathrm{H}}_n(x)$$
$$= \sum_{n=0}^{N} \left(\hat{f}_n(t) - \hat{f}_{\Delta,n}(t)\right)\tilde{\mathrm{H}}_n(x) + \sum_{n=N+1}^{\infty} \hat{f}_n(t)\tilde{\mathrm{H}}_n(x).$$

From Lemma 1 we know that the first term in the last line of the equation above is zero; hence Lemma 3 gives us the following bound for the error:

$$\|f(\cdot,t) - f_\Delta(\cdot,t)\|^2_{w_\alpha} = \int_{\mathbb{R}} \left[\sum_{n=N+1}^{\infty} \hat{f}_n(t)\tilde{\mathrm{H}}_n(x)\right]^2 w(x)dx$$
$$= \frac{\sqrt{\pi}}{\alpha} \sum_{n=N+1}^{\infty} |\hat{f}_n(t)|^2$$
$$\leq \frac{\sqrt{\pi}}{\alpha} \sum_{n=N+1}^{\infty} \frac{\alpha^{2-2r}}{\pi} n^{-r} \|f(\cdot,t)\|^2_{r,w_\alpha}.$$

Therefore, we have $\|f(\cdot,t) - f_\Delta(\cdot,t)\|^2_{w_\alpha} = O(N^{-r})$. □

The following lemma provides an appropriate means to show that the Hermite discretization method is stable.

Lemma 2. *Let M be the $(N+1)\times(N+1)$ matrix M_f or M_q, and let $\hat{y}(t)$ be the solution to*

$$\frac{d}{dt}\hat{y}(t) = M\hat{y}, \qquad \hat{y}(0) = \hat{y}_0.$$

Then there exists a constant C_N such that for all $t > 0$

$$\|\hat{y}(t)\|_2 \leq C_N \|\hat{y}_0\|_2.$$

Proof. Since the matrix M is triangular, it has $N+1$ distinct eigenvalues $\lambda_n = n\gamma$, $n = 0,1,\cdots,N$, which are the diagonal elements of M. Therefore, M is diagonalizable and can be decomposed as $M = S^{-1}DS$, where $D = \mathrm{diag}(\lambda_n)_{n=0}^N$. Hence, the system of ODEs has the solution

$$\hat{y}(t) = e^{Mt}\hat{y}_0,$$

which implies the following:

$$\|\hat{y}(t)\|_2 \leq \|S^{-1}\|_2 \|e^{Dt}\|_2 \|S\|_2 \|\hat{y}_0\|_2.$$

Since $\gamma < 0$, we have $e^{2\lambda_n t} \leq 1$, $n = 0,1,\cdots,N$, and consequently

$$\|e^{Dt}\|_2 = \sigma_{\max}(e^{Dt}) = \sqrt{\lambda_{\max}(e^{2Dt})} \leq 1.$$

It is easy to show that the matrices S and S^{-1} have the same structure as the matrix M. That is, they are lower triangular when M is lower triangular, and upper triangular when M is upper triangular. Since S is consists of the eigenvectors of M, it can be constructed in such a way that all diagonal elements are 1. Defining $\tilde{s} := \|S\|_{\max} = \max_{1\leq i,j\leq N+1} |S_{ij}|$ we have

$$\|S\|_2 \leq (N+1)\|S\|_{\max} = (N+1)\tilde{s}.$$

Furthermore, in [15] it is proved that

$$\|S^{-1}\|_\infty \le (\tilde{s}+1)^N,$$

which results in

$$\|S^{-1}\|_2 \le \sqrt{N+1}\|S^{-1}\|_\infty \le \sqrt{N+1}(\tilde{s}+1)^N.$$

Therefore, we have

$$\|\hat{y}(t)\|_2 \le C_N\|\hat{y}_0\|_2.$$

where $C_N = (N+1)^{3/2}(\tilde{s}+1)^{N+1}$.

□

Based on Lemma 2, we have the following stability result.

Theorem 4. *There exists a constant C_N such that for all $t > 0$*

$$\|f_\Delta(.,t)\|_{w_\alpha} \le C_N\|\hat{f}_0\|_2, \quad \textit{and} \quad \|p_\Delta(.,t)\|_{w_\alpha} \le C_N\|\hat{p}_0\|_2.$$

Proof. We only prove the inequality for f_Δ, since the argument is the same for p_Δ. We have

$$\begin{aligned}
\|f_\Delta(.,t)\|^2_{w_\alpha} &= \int_{\mathbb{R}} (f_\Delta)^2 w_\alpha(x)dx = \int_{\mathbb{R}} \left(\sum_{n=0}^{N} \hat{f}_{\Delta,n}(t)\tilde{\mathrm{H}}_n(x)\right)^2 w_\alpha(x)dx \\
&= \frac{\sqrt{\pi}}{\alpha}\sum_{n=0}^{N}(\hat{f}_{\Delta,n}(t))^2 = \frac{\sqrt{\pi}}{\alpha}\|\hat{f}_\Delta(t)\|_2^2 \le C\|\hat{f}_0\|_2^2.
\end{aligned}$$

□

Now we investigate the spectral convergence in approximating the control variable.

Theorem 5. *Let $f \in L^\infty(0,T;H^r_{w_\alpha}(\mathbb{R}))$, $r > 2$ and $N \ge 2$. Then for a positive constant c, we have*

$$|u - u_\Delta| \le cT\sum_{n=N}^{\infty} n^{1-r}.$$

Proof. We start from optimality equations in the continuous and discrete form:

$$\nu u + \int_0^T \int_{\mathbb{R}} (\partial_x f)\, p\, w_\alpha\, dx\, dt = 0,$$

$$\nu u_\Delta + \int_0^T \int_{\mathbb{R}} (\partial_x f_\Delta)\, p_\Delta\, w_\alpha\, dx\, dt = 0.$$

We note that

$$\begin{aligned}
\int_{\mathbb{R}} (\partial_x f) p w_\alpha dx &= \int_{\mathbb{R}} \left(\sum_{n=0}^{\infty} \hat{f}_n \partial_x \tilde{\mathrm{H}}_n(x)\right)\left(\sum_{n=0}^{\infty} \hat{p}_n \tilde{\mathrm{H}}_n(x)\right) w_\alpha dx \\
&= -\alpha \int_{\mathbb{R}} \left(\sum_{n=0}^{\infty} \sqrt{2(n+1)}\hat{f}_n \tilde{\mathrm{H}}_{n+1}(x)\right)\left(\sum_{n=0}^{\infty} \hat{p}_n \tilde{\mathrm{H}}_n(x)\right) w_\alpha dx \\
&= -\alpha \sum_{n=0}^{\infty}\sum_{k=0}^{\infty} \sqrt{2(n+1)}\hat{f}_n \hat{p}_k \int_{\mathbb{R}} \tilde{\mathrm{H}}_{n+1}(x)\tilde{\mathrm{H}}_k(x) w_\alpha dx \\
&= -\alpha \sum_{n=0}^{\infty} \sqrt{2(n+1)}\hat{f}_n \hat{p}_{n+1}\frac{\sqrt{\pi}}{\alpha} \\
&= -\sum_{n=0}^{\infty} \sqrt{2\pi(n+1)}\hat{f}_n \hat{p}_{n+1}.
\end{aligned}$$

Similarly, we have

$$\int_{\mathbb{R}} (\partial_x f_\Delta) p_\Delta w_\alpha dx = -\sum_{n=0}^{N-1} \sqrt{2\pi(n+1)} \hat{f}_{\Delta,n} \hat{p}_{\Delta,n+1}.$$

Therefore,

$$\begin{aligned} -\left(\int_{\mathbb{R}} (\partial_x f) p w_\alpha dx - \int_{\mathbb{R}} (\partial_x f_\Delta) p_\Delta w_\alpha dx \right) &= \sum_{n=0}^{\infty} \sqrt{2\pi(n+1)} \hat{f}_n \hat{p}_{n+1} - \sum_{n=0}^{N-1} \sqrt{2\pi(n+1)} \hat{f}_{\Delta,n} \hat{p}_{\Delta,n+1} \\ &= \sum_{n=0}^{N-1} \sqrt{2\pi(n+1)} \left(\hat{f}_n \hat{p}_{n+1} - \hat{f}_{\Delta,n} \hat{p}_{\Delta,n+1} \right) \\ &+ \sum_{n=N}^{\infty} \sqrt{2\pi(n+1)} \hat{f}_n \hat{p}_{n+1}. \end{aligned}$$

Noting that

$$\begin{aligned} \hat{f}_n \hat{p}_{n+1} - \hat{f}_{\Delta,n} \hat{p}_{\Delta,n+1} &= \hat{f}_n \hat{p}_{n+1} - \hat{f}_n \hat{p}_{\Delta,n+1} + \hat{f}_n \hat{p}_{\Delta,n+1} - \hat{f}_{\Delta,n} \hat{p}_{\Delta,n+1} \\ &= \hat{f}_n \left(\hat{p}_{n+1} - \hat{p}_{\Delta,n+1} \right) + \hat{p}_{\Delta,n+1} \left(\hat{f}_n - \hat{f}_{\Delta,n} \right), \end{aligned}$$

we can write

$$\begin{aligned} \frac{1}{\sqrt{2\pi}} \left| \int_{\mathbb{R}} (\partial_x f) p w_\alpha dx - \int_{\mathbb{R}} (\partial_x f_\Delta) p_\Delta w_\alpha dx \right| &\leq \sum_{n=0}^{N-1} \sqrt{n+1} |\hat{f}_n| . |\hat{p}_{n+1} - \hat{p}_{\Delta,n+1}| \\ &+ \sum_{n=0}^{N-1} \sqrt{n+1} |\hat{p}_{\Delta,n+1}| . |\hat{f}_n - \hat{f}_{\Delta,n}| \\ &+ \sum_{n=N}^{\infty} \sqrt{n+1} |\hat{f}_n| . |\hat{p}_{n+1}|. \end{aligned}$$

From Lemma 1, we have

$$\sum_{n=0}^{N} |\hat{f}_n - \hat{f}_{\Delta,n}|^2 = 0, \qquad \text{and} \qquad \sum_{n=0}^{N} |\hat{p}_{\Delta,n} - \hat{p}_n|^2 = 0,$$

which implies that $|\hat{f}_n - \hat{f}_{\Delta,n}| = 0$ and $|\hat{p}_{\Delta,n} - \hat{p}_n| = 0$ for $n = 0, 1, \cdots, N$. Hence

$$\frac{1}{\sqrt{2\pi}} | \int_{\mathbb{R}} (\partial_x f) p w_\alpha dx - \int_{\mathbb{R}} (\partial_x f_\Delta) p_\Delta w_\alpha dx | \leq \sum_{n=N}^{\infty} \sqrt{n+1} |\hat{f}_n| . |\hat{p}_{n+1}|.$$

Assuming $N \geq 2$, Lemma 3 gives us

$$\begin{aligned} \sum_{n=N}^{\infty} \sqrt{n+1} |\hat{f}_n| . |\hat{p}_{n+1}| &\leq \sum_{n=N}^{\infty} \sqrt{n+1} \left(\frac{\alpha^{1-r}}{\sqrt{\pi}} \right)^2 n^{-r/2} (n+1)^{-r/2} \|f\|_{r,w_\alpha} \|p\|_{r,w_\alpha} \\ &\leq c_{fp} \sum_{n=N}^{\infty} n \, n^{-r/2} n^{-r/2} = c_{fp} \sum_{n=N}^{\infty} n^{1-r}, \end{aligned}$$

in which $c_{fp} = (\alpha^{2-2r})/\pi \|f\|_{r,w_\alpha} \|p\|_{r,w_\alpha}$. Therefore, the desired accuracy estimate for the control variable u can be written as follows

$$|u - u_\Delta| \leq c T \sum_{n=N}^{\infty} n^{1-r},$$

where $c = \sqrt{2\pi}/\nu c_{fp}$. □

An important property of the numerical scheme is that the Hermite spectral discretization provides conservativeness. We prove the following:

$$\int_{\mathbb{R}} f_\Delta(x,t)dx = \int_{\mathbb{R}} f_\Delta(x,0)dx, \qquad t > 0.$$

First, we note that for any $t > 0$,

$$\begin{aligned}\int_{\mathbb{R}} f_\Delta(x,t)dx &= \sum_{n=0}^{N} \hat{f}_{\Delta,n}(t) \int_{\mathbb{R}} \tilde{\mathrm{H}}_n(x)\, dx \\ &= \hat{f}_{\Delta,0}(t) \int_{\mathbb{R}} \tilde{\mathrm{H}}_0(x)\, dx.\end{aligned}$$

This is true because of Lemma 4 which states that $\int_{\mathbb{R}} \tilde{\mathrm{H}}_n(x)dx = 0$ for $n \geq 1$.

Noting that $d\hat{f}_\Delta/dt = M_f \hat{f}_\Delta$, and the fact that the first row of the matrix M_f is zero, we have

$$\hat{f}_{\Delta,0}(t) = \hat{f}_{\Delta,0}(0), \qquad t > 0.$$

Therefore, we have

$$\begin{aligned}\int_{\mathbb{R}} f_\Delta(x,t)dx &= \hat{f}_{\Delta,0}(t) \int_{\mathbb{R}} \tilde{\mathrm{H}}_0(x)\, dx \\ &= \hat{f}_{\Delta,0}(0) \int_{\mathbb{R}} \tilde{\mathrm{H}}_0(x)\, dx \\ &= \sum_{n=0}^{N} \hat{f}_{\Delta,n}(0) \int_{\mathbb{R}} \tilde{\mathrm{H}}_n(x)\, dx \\ &= \int_{\mathbb{R}} f_\Delta(x,0)\, dx.\end{aligned}$$

6. NUMERICAL EXPERIMENTS

Since the system of ODEs which we need to solve in order to obtain the numerical solutions are first-order linear systems, there exists no time discretization in our numerical scheme. That is, we can calculate the Hermite expansion coefficients analytically and without any time discretization error. The triangular structure of the matrices of coefficients with distinct eigenvalues makes it possible to decompose the mentioned matrices and solve the system of ODEs simply by matrix products. Therefore, the errors presented in this section are only induced by spatial discretization.

In [9] it is stated that the Hermite spectral method does not provide good resolution for all scaling factor α. It is thence proved that to approximate Gaussian-type functions e^{-sx^2}, the scaling factor α must satisfy $0 < \alpha < \sqrt{2s}$. Consider the forward FP equation

$$\partial_t f(x,t) - c\partial_{xx} f(x,t) + \partial_x \left((\gamma x + u) f(x,t)\right) = 0.$$

It is easy to see that the stationary solution, which satisfies $\partial_t f = 0$, or equivalently

$$\partial_x \left(c\partial_x f - (\gamma x + u) f\right) = 0,$$

is as follows:

$$f(x) = C_0 \exp\left(\frac{\gamma}{2c}x^2 + \frac{u}{c}x\right),$$

where C_0 is a constant. Comparing the stationary solution with the weight function $w_\alpha(x)$, while the control variable $u = 0$, motivates us to set $\alpha = \sqrt{-\gamma/2c}$. This choice satisfies the condition mentioned in [9], and seems to be the best option since to find the optimal scaling factor is still an open problem.

To illustrate the importance of choosing a proper scaling factor, consider Case 1 with a known exact solution for the following FP equation:

$$\partial_t f - \partial_{xx} f - \partial_x (xf) = 0,$$

with the initial condition

$$f(x,0) = e^{[-(x^2/2)]} \left(1 + \cos[(\pi/2)x] \exp[\pi^2/8]\right).$$

The exact solution of this problem is given by

$$f(x,t) = e^{[-(x^2/2)]} \left(1 + \cos[(\pi/2)xe^{-t}] \exp[\pi^2/8]e^{-2t}\right).$$

Since the parameters of the FP equation are $c = 1$, $\gamma = -1$, and $u = 0$, we set $\alpha := \sqrt{-\gamma/2c} = 1/\sqrt{2} \approx 0.7071$. Figure 1 illustrates how different values for the scaling factor may lead to different approximations for a given N. However, as mentioned in [9] the Hermite approximation is accurate in solving for the asymptotic solution also without an optimal α.

In Table 1, we see how fast the error decreases when t increases. After reaching to the equilibrium solution the error remains at the value of the machine error. We can investigate more about Hermite discretization with this experiment. Table 2 shows the decay of the error regarding increasing N.

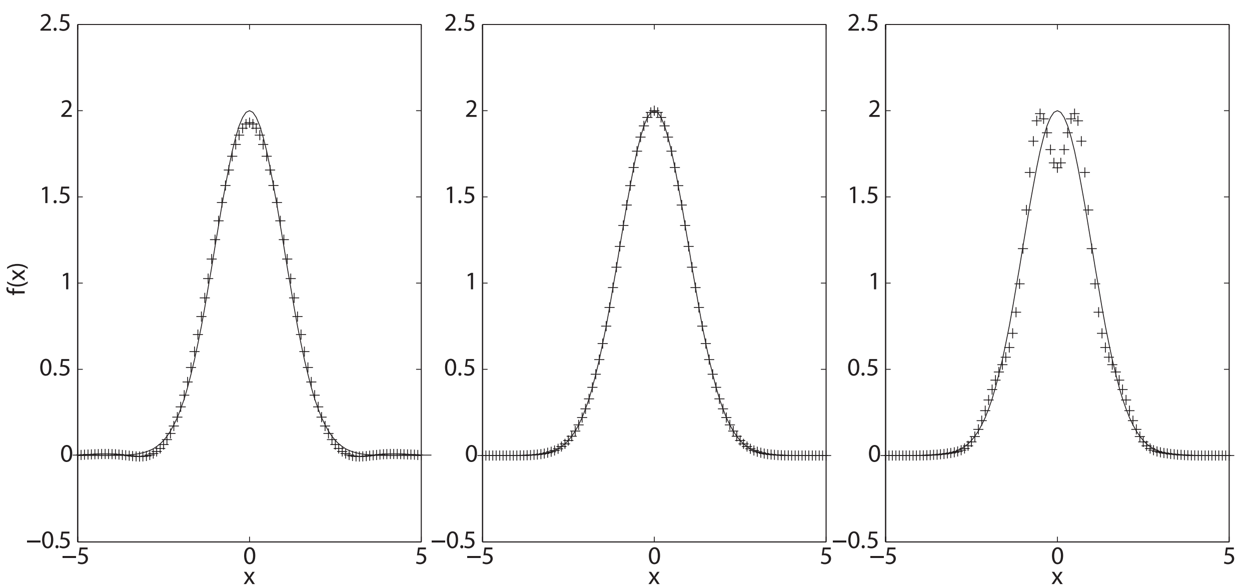

FIG. 1: Case 1: numerical (cross-marks) and exact solution (solid line) to the FP equation with different scaling factors; left: $\alpha = 0.4$, middle: $\alpha = 0.7071$, right: $\alpha = 1$; $N = 10$ and $T = 10$.

TABLE 1: Case 1: decay of the solution error at final time when T increases; $N = 10$, $\alpha = 0.7071$

T	$\|f_\Delta - f_{exact}\|_{L^2}$
1	2.0101e-11
2	1.2132e-16
3	3.0412e-18
4	3.0428e-18
5	3.0450e-18

TABLE 2: Decay of the error in case 1 when N increases; $T = 1$, $\alpha = 0.7071$

N	$\|f_\Delta - f_{exact}\|_{L^2}$
5	4.2193e-07
10	2.0101e-11
15	1.0275e-14
20	2.9166e-18

Since in our Hermite spectral discretization, the initial condition of the differential equation has to be mapped into the approximation space V_N, if N is not large enough to have a precise representation of the initial data, one cannot expect a satisfactory numerical result. However, in Fig. 2 we see that for the problems dealing with a Gaussian-type function, the influence of the error in representing the initial data becomes negligible along time evolution.

Next, we extend the experiment to an optimal control problem and consider Case 2. We set $c = 1$, $\gamma = -1$, $\nu = 0.1$, $T = 1$, and introduce the following initial condition for the FP equation:

$$\rho(x) = e^{[-(x^2/2)]}\left(1 + \cos[(\pi/2)x]\exp[\pi^2/8]\right).$$

In order to make it possible to illustrate the spectral accuracy of the adjoint and the control variables, we insert the desired function

$$f_d(x,t) = e^{[-(x^2/2)]}\left(1 + \cos[(\pi/2)xe^{-t}]\exp[\pi^2/8]e^{-2t}\right)$$

into the optimality system, which is the same as the solution of the forward FP equation. With this setting, the exact solution of the optimality system is given by $f = f_d$, $p = 0$, and $u = 0$. We apply our spectral discretization for this optimality system, and obtain very accurate numerical approximations; see Table 3 for the norm of the solution errors. We observe that the Hermite spectral method converges spectrally and is very accurate even for small N.

In Case 3, we impose the PDF to follow a desired function which is a Gaussian with a varying center. The control variable then must vary in order to keep the PDF as close as possible to the desired function. Let $\nu = 0.1$,

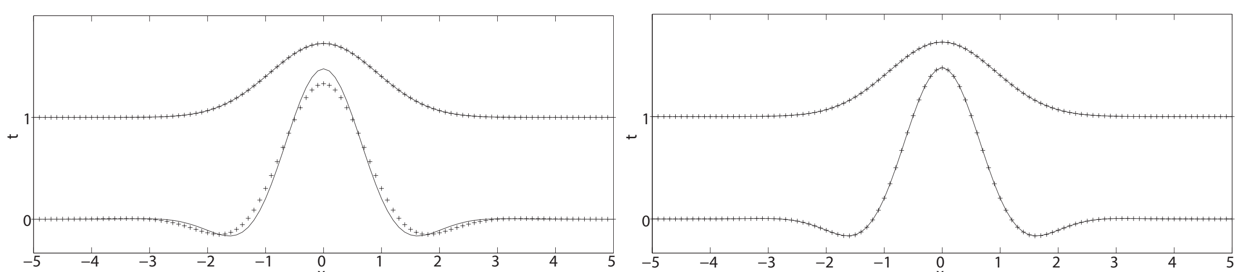

FIG. 2: Case 1: Accurate approximation for the solution at $T = 1$ (top graph), even if the initial solution is not well approximated (bottom graph). Left figure: $N = 5$, right figure: $N = 10$. Cross-marks represent the numerical solution and the solid lines represent the exact solution.

TABLE 3: Case 2: Accurate approximation results of the optimality system for different N

N	$\|f_\Delta - f_{exact}\|_{L^2}$	$\|p_\Delta - p_{exact}\|_{L^2}$	$\|u_\Delta - u_{exact}\|$
5	1.6858e-05	5.3832e-15	2.1653e-16
10	6.8641e-10	5.3836e-15	5.9684e-16
15	4.3062e-13	5.3870e-15	2.1858e-15
20	1.0100e-14	5.9588e-15	1.5715e-16

$$f_d(x,t) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x - 2\sin(\pi t/5))^2}{2\sigma^2}\right)$$

with $\sigma = 0.2$, and consider the following setting for the evolution of PDF. The initial PDF is

$$f_0(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right)$$

with $\sigma = 0.5$, and the parameters in the forward equation are $\gamma = -1$, $c = 0.32$. We consider a model predictive control scheme, which is introduced in [2], to track f_d by the PDF. In this control scheme, we divide the time interval $[0, T]$ into k subintervals, and solve the optimization problem for any time window of size $\Delta t = T/k$. At any time window $(t_k, t_{k+1}]$ an optimal control u imposes the PDF of that window to evolve towards the desired function $f_d(x, t_{k+1})$. While for a given u, the state and the adjoint variables are approximated directly with the Hermite spectral method, we employ the nonlinear conjugate gradient scheme proposed in [2] to evaluate the optimal control u. The final PDF of a window is considered to be the initial solution of the next window. Figure 3 along with Table 4 show

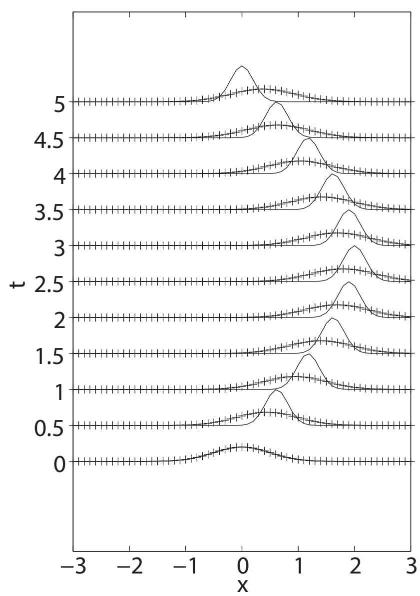

FIG. 3: Case 3: Approximated solution of FP equation (cross-marks) tracking the desired PDF (solid line) at different time windows.

TABLE 4: Case 3: The optimal control variable u at different time windows

Time interval	u
(0,0.5]	1.1374
(0.5,1]	1.7166
(1,1.5]	2.0767
(1.5,2]	2.1216
(2,2.5]	1.9601
(2.5,3]	1.5307
(3,3.5]	0.9934
(3.5,4]	0.4265
(4,4.5]	0.0019
(4.5,5]	0.0000

the outcome of this control strategy. In this experiment, $\Delta t = 0.5$, $\alpha = 0.7$, and $N = 50$. With this setting, it takes around 10 minutes to obtain the numerical solution by MATLAB.

Finally, to examine the Hermite discretization scheme concerning conservativity, we introduce Case 4. In this experiment, we can also compare the approximated solution with the exact solution of an FP equation with a non-zero u, which is presented in [1]. The exact solution of the FP equation

$$\partial_t f(x,t) - c\partial_{xx} f(x,t) + \partial_x \left((\gamma x + u) f(x,t)\right) = 0$$

with the initial condition

$$f_0(x) = \delta(x)$$

is a Gaussian distribution with mean $\mu(t,u) = -u/\gamma + (u/\gamma)e^{\gamma t}$ and variance $\bar{\sigma}^2(t) = -c/\gamma(1 - e^{2\gamma t})$; that is

$$f(x,t,u) = \frac{1}{\sqrt{2\pi\bar{\sigma}^2(t)}} \exp\left(-\frac{(x - \mu(t,u))^2}{2\bar{\sigma}^2(t)}\right).$$

Since it is impossible to represent the Dirac delta function $\delta(0)$ by Hermite functions, we apply a temporal shift in the exact solution in order to have a Gaussian function as the initial condition. In Fig. 4, time $t = 1$ has been considered to be the starting time of the process which evolves under the action of the control $u = 2$. We observe how fast the approximation becomes accurate as N increases.

Since in this case, $u \neq 0$ and consequently the stationary solution is not centered at zero, it becomes harder to deal with a proper choice of the scaling factor α. By trying different values of α, we gain the best estimate corresponding to $\alpha = 0.7$. However, the error estimate presented in Table 5 is not as perfect as the estimation in Case 1, which is

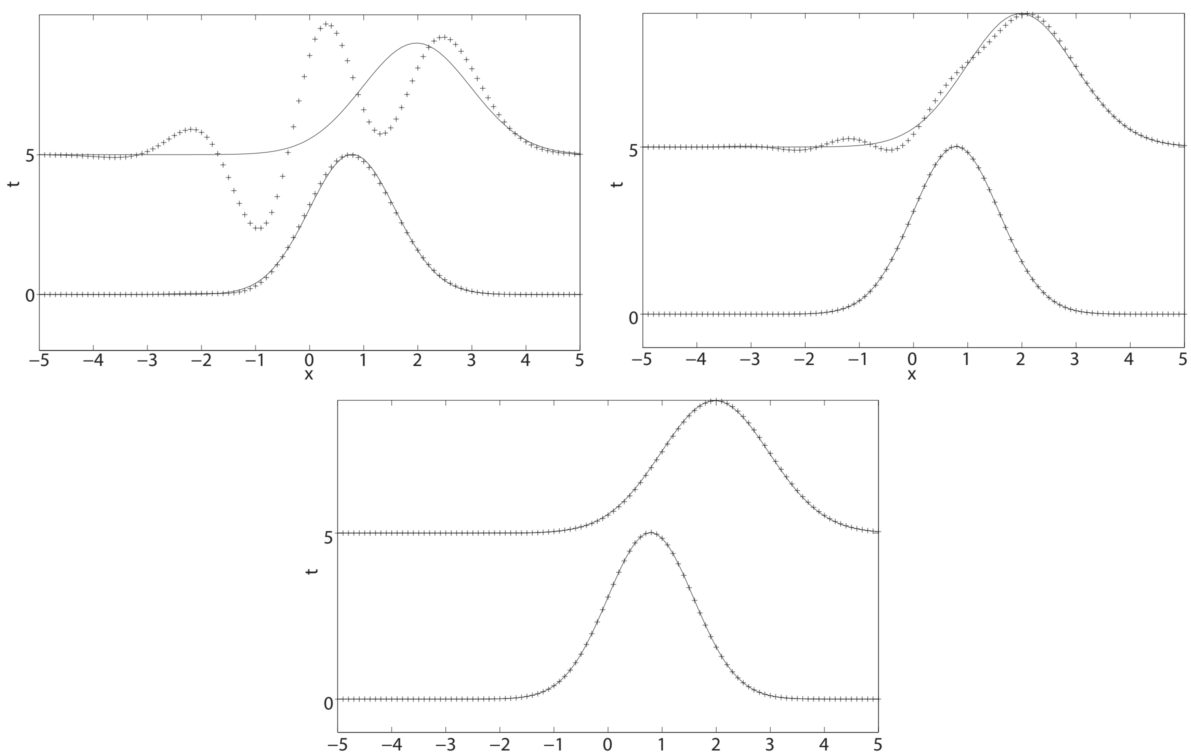

FIG. 4: Case 4: Approximations of the initial PDF and the solution at $T = 5$. Left figure: $N = 5$, right figure: $N = 10$, bottom figure: $N = 15$. Cross-marks represent the numerical solution and the solid lines represent the exact solution.

TABLE 5: Case 4: Positivity and conservativity of Hermite discretization

N	Error	$\min_{x\in\mathbb{R}} f_\Delta(x,0)$	$\min_{x\in\mathbb{R}} f_\Delta(x,5)$	$\int_\mathbb{R} f_\Delta(x,0)dx$	$\int_\mathbb{R} f_\Delta(x,5)dx$
5	0.4307	–3.1391e-04	–0.2628	1.0000	1.0000
10	0.0403	–5.8202e-05	–0.0095	1.0000	1.0000
15	0.0054	–2.3574e-06	–8.5076e-05	1.0000	1.0000
20	0.0053	–2.7610e-08	–2.5495e-07	1.0000	1.0000
25	0.0053	–7.8068e-10	–1.2459e-11	1.0000	1.0000
30	0.0053	–2.9185e-11	0	1.0000	1.0000

due to considering a constant scaling factor instead of a time-dependent one. The idea of the time-dependent scaling factor is discussed in [18], while one can also think about inserting a translating factor into the Hermite functions to treat the non-zero-centered Gaussian functions. This strategy is applied in [17].

Further, Table 5 verifies that when the number of the expansion terms is large enough to have an almost non-negative representation of the initial PDF, the discretization scheme leads to an almost non-negative solution of the forward FP equation. We observe that the property $\int_\mathbb{R} f(x,t) = 1$, $t \geq 0$, is perfectly preserved independent of the number of expansion terms.

7. CONCLUSION

A Hermite spectral discretization method to approximate the solution of a Fokker-Planck optimal control problem in an unbounded domain was presented. It was proved that the resulting numerical solution is spectrally accurate for all unknown variables of the optimality system. Moreover, it was proved that the proposed discretization scheme preserves conservativity of the solution. Since a weighted Hermite approximation method was used, the optimal choice for the scaling factor in the weight function was investigated with numerical experiments. Results of numerical experiments demonstrated the theoretical estimates.

APPENDIX A. HERMITE APPROXIMATION SPACE

Hermite functions are defined as follows:

$$\tilde{\mathrm{H}}_n(x) = \frac{1}{\sqrt{2^n n!}} H_n(\alpha x) w_\alpha^{-1}(x), \quad \alpha > 0, \quad n \geq 0,$$

where $w_\alpha(x) = \exp(\alpha^2 x^2)$ is a weight function and H_n is the Hermite polynomial of degree n given by

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n}(e^{-x^2}).$$

We introduce the following inner product and the associated norm:

$$(y,z)_{w_\alpha} = \int_\mathbb{R} y(x)z(x)w_\alpha(x)dx, \quad \|y\|_{w_\alpha} = (y,y)_{w_\alpha}^{1/2}, \qquad y,z \in L^2_{w_\alpha}(\mathbb{R}),$$

and also consider the weighted Sobolev space

$$H^r_{w_\alpha}(\mathbb{R}) = \left\{ y \mid \frac{d^k y}{dx^k} \in L^2_{w_\alpha}(\mathbb{R}),\ 0 \leq k \leq r \right\},$$

equipped with the following semi-norm and norm, respectively,

$$|y|_{k,w_\alpha} = \left\| \frac{d^k y}{dx^k} \right\|_{w_\alpha}, \quad \|y\|_{r,w_\alpha} = \left(\sum_{k=0}^{r} |y|^2_{k,w_\alpha} \right)^{1/2}.$$

We note that the set of functions $\{\tilde{\text{H}}_n(x), n \geq 0\}$ defines a $L^2_{w_\alpha}(\mathbb{R})$-orthogonal system with

$$(\tilde{\text{H}}_n, \tilde{\text{H}}_m)_{w_\alpha} = \frac{\sqrt{\pi}}{\alpha}\delta_{n,m},$$

where $\delta_{n,m}$ is the Kronecker delta. Therefore for all $y \in L^2_{w_\alpha}(\mathbb{R})$, we can write

$$y(x) = \sum_{n=0}^{\infty} \hat{y}_n \tilde{\text{H}}_n(x),$$

with the coefficients

$$\hat{y}_n = \frac{\alpha}{\sqrt{\pi}} \int_{\mathbb{R}} y(x)\tilde{\text{H}}_n(x) w_\alpha(x) dx, \quad n \geq 0.$$

We define

$$V_N = \{q(x)w_\alpha^{-1}(x) \,|\, q(x) \in \mathbb{P}_N\},$$

and note that $V_N = \text{span}\{\tilde{\text{H}}_n(x),\ 0 \leq n \leq N\}$, where $\mathbb{P}_N$ is the set of polynomials of degree at most N. Therefore we can consider the $L^2_{w_\alpha}(\mathbb{R})$-orthogonal projection $P_N : L^2_{w_\alpha}(\mathbb{R}) \to V_N$, with

$$P_N y(x) = \sum_{n=0}^{N} \hat{y}_n \tilde{\text{H}}_n(x).$$

In [9] the following theorem is proved, which is used in our work to estimate the approximation error in the space V_N.

Theorem 6. *For any $y \in H^r_{w_\alpha}(\mathbb{R})$ and $r \geq 0$,*

$$\|y - P_N y\|_{w_\alpha} \leq c(\alpha^2 N)^{-r/2} \|y\|_{r,w_\alpha},$$

where $c = (\alpha/2^r\sqrt{\pi})^{1/2}$.

This theorem also helps us to estimate the Hermite coefficients. We prove the following lemma.

Lemma 3. *For any $y \in H^r_{w_\alpha}(\mathbb{R})$, $r \geq 0$, and $n \geq 2$,*

$$|\hat{y}_n(t)| \leq \frac{\alpha^{1-r}}{\sqrt{\pi}} n^{-r/2} \|y(.,t)\|_{r,w_\alpha}.$$

Proof. Considering $n \geq 1$ and the orthogonality relation between Hermite functions, we can write the following inequality:

$$\begin{aligned} |\hat{y}_n(t)|^2 &\leq \sum_{k=n}^{\infty} |\hat{y}_k(t)|^2 = \frac{\alpha}{\sqrt{\pi}} \sum_{k=n}^{\infty} \frac{\sqrt{\pi}}{\alpha} |\hat{y}_k(t)|^2 = \frac{\alpha}{\sqrt{\pi}} \int_{\mathbb{R}} \left(\sum_{k=n}^{\infty} \hat{y}_k(t) \tilde{\text{H}}_k(v) \right)^2 w_\alpha(v) dv \\ &= \frac{\alpha}{\sqrt{\pi}} \int_{\mathbb{R}} \left(\sum_{k=0}^{\infty} \hat{y}_k(t)\tilde{\text{H}}_k(v) - \sum_{k=0}^{n-1} \hat{y}_k(t)\tilde{\text{H}}_k(v) \right)^2 w_\alpha(v) dv \\ &= \frac{\alpha}{\sqrt{\pi}} \|y - P_{n-1} y\|^2_{w_\alpha}. \end{aligned}$$

By Theorem 6, we have

$$\|y - P_{n-1}y\|_{w_\alpha} \leq \left(\frac{\alpha}{2^r\sqrt{\pi}} \right)^{1/2} (\alpha^2(n-1))^{-r/2} \|y\|_{r,w_\alpha}.$$

Therefore,

$$|\hat{y}_n(t)| \leq \frac{2^{-r/2}}{\sqrt{\pi}} \alpha^{1-r}(n-1)^{-r/2} \|y(.,t)\|_{r,w_\alpha}.$$

Since for $n \geq 2$ we have $2(n-1) \geq n$, and consequently $2^{-r/2}(n-1)^{-r/2} \leq n^{-r/2}$, the following holds for $n \geq 2$:

$$|\hat{y}_n(t)| \leq \frac{\alpha^{1-r}}{\sqrt{\pi}} n^{-r/2} \|y(.,t)\|_{r,w_\alpha}.$$

□

To discretize the FP equation, we employ the following facts:

$$\alpha x \tilde{\mathrm{H}}_n(x) = \sqrt{\frac{n+1}{2}}\ \tilde{\mathrm{H}}_{n+1}(x) + \sqrt{\frac{n}{2}}\ \tilde{\mathrm{H}}_{n-1}(x),$$

$$\frac{d}{dx}\tilde{\mathrm{H}}_n(x) = -\alpha\sqrt{2(n+1)}\ \tilde{\mathrm{H}}_{n+1}(x),$$

$$x\frac{d}{dx}\tilde{\mathrm{H}}_n(x) = -\sqrt{(n+1)(n+2)}\ \tilde{\mathrm{H}}_{n+2}(x) - (n+1)\tilde{\mathrm{H}}_n(x),$$

$$\frac{d^2}{dx^2}\tilde{\mathrm{H}}_n(x) = 2\alpha^2\sqrt{(n+1)(n+2)}\ \tilde{\mathrm{H}}_{n+2}(x),$$

for $n \geq 0$, with $\tilde{\mathrm{H}}_j(x) = 0, j < 0$.

We also have

$$xH_n(x) = \frac{1}{2}H_{n+1}(x) + nH_{n-1}(x),$$

$$\frac{d}{dx}H_n(x) = 2nH_{n-1}(x),$$

$$x\frac{d}{dx}H_n(x) = nH_n(x) + 2n(n-1)H_{n-2}(x),$$

$$\frac{d^2}{dx^2}H_n(x) = 4n(n-1)H_{n-2}(x),$$

or equivalently,

$$\alpha x H_n(\alpha x) = \frac{1}{2}H_{n+1}(\alpha x) + nH_{n-1}(\alpha x),$$

$$\frac{d}{dx}H_n(\alpha x) = 2\alpha n H_{n-1}(\alpha x),$$

$$x\frac{d}{dx}H_n(\alpha x) = nH_n(\alpha x) + 2n(n-1)H_{n-2}(\alpha x),$$

$$\frac{d^2}{dx^2}H_n(\alpha x) = 4\alpha^2 n(n-1)H_{n-2}(\alpha x).$$

which provide the appropriate means to descretize the optimal control system.

We also prove the following lemma to discuss the conservativity of the discretized FP equation.

Lemma 4. *For* $n \geq 1$

$$\int_{\mathbb{R}} \tilde{H}_n(x)dx = 0.$$

Proof. Based on

$$\tilde{\mathrm{H}}_n(-x) = (-1)^n \tilde{\mathrm{H}}_n(x),$$

we see that $\tilde{\mathrm{H}}_n$ is an even function when n is even, and it is an odd function when n is odd. Therefore, it is clear that $\int_{\mathbb{R}} \tilde{\mathrm{H}}_n(x)dx = 0$ when n is odd. Assuming that n is even, and using the following fact,

$$\int_0^x e^{-t^2} H_n(t)dt = H_{n-1}(0) - e^{-x^2} H_{n-1}(x),$$

we obtain

$$\begin{aligned}
\int_{\mathbb{R}} \tilde{\mathrm{H}}_n(x)dx &= \frac{1}{\sqrt{2^n n!}} \int_{\mathbb{R}} H_n(\alpha x) e^{-\alpha^2 x^2} dx \\
&= \frac{1}{\alpha\sqrt{2^n n!}} \int_{\mathbb{R}} H_n(t) e^{-t^2} dt \\
&= \frac{1}{\alpha\sqrt{2^n n!}} \left(\int_{-\infty}^0 H_n(t) e^{-t^2} dt + \int_0^\infty H_n(t) e^{-t^2} dt \right) \\
&= \frac{2}{\alpha\sqrt{2^n n!}} \lim_{x\to\infty} \int_0^x H_n(t) e^{-t^2} dt \\
&= \frac{2}{\alpha\sqrt{2^n n!}} \lim_{x\to\infty} \left(H_{n-1}(0) - e^{-x^2} H_{n-1}(x) \right).
\end{aligned}$$

Since H_{n-1} is an odd function, $H_{n-1}(0) = 0$ and the desired statement is proved. □

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