ANALYSIS OF AN OPTIMAL CONTROL PROBLEM OF THE BACKWARD FRACTIONAL FEYNMAN-KAC EQUATION WITH TEMPORAL APPROXIMATION*

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Abstract. In this paper, we discuss an optimal control problem governed by the backward fractional Feynman-Kac equation, which depicts the probability density function of functionals of widespread diffusion phenomena in various multiscale fields. In the constrained equation, the time-space coupled nonlocal operator and its noncommutativity with Laplacian bring significant difficulties. The well-posedness, optimality conditions and solution's regularity of the continuous optimal control problem are established. Then, we propose a temporal semidiscrete scheme for the optimal control problem by applying the backward Euler convolution quadrature (BECQ) formula to discretize the Riemann-Liouville fractional substantial derivative in the equation. In addition, the error estimate of the proposed semidiscrete scheme is rigorously established, and almost optimal convergence of $O(\tau|\ln \tau|)$ is obtained depending only on the regularity assumptions on the data and without extra assumptions on the solution. Some numerical examples are illustrated to verify the theoretical results.

Keywords. optimal control problem, backward fractional Feynman-Kac equation, fractional substantial derivative, convolution quadrature, error estimate

AMS subject classifications. 49K20, 49M25, 35R11, 65M12

1. Introduction.

Let Ω be a bounded convex polygonal domain with the boundary $\partial\Omega$ in $\mathbb{R}^d$, $d \geq 1$. We consider to design and analyze a temporal semidiscrete scheme for the optimal control problem:

$$\min_{q\in U_{ad}} J(u,q) = \frac{1}{2}\|u-u_d\|^2_{L^2(0,T;L^2(\Omega))} + \frac{\gamma}{2}\|q\|^2_{L^2(0,T;L^2(\Omega))}, \tag{1.1}$$

subject to the backward fractional Feynman-Kac equation [2, 34]

$$\begin{cases} \partial_t u(x,t) - D_t^{1-\alpha,x}\Delta u(x,t) + \rho U(x)u(x,t) = f(x,t)+q(x,t), & (x,t)\in\Omega\times(0,T],\\ u(x,t)=0, & (x,t)\in\partial\Omega\times(0,T],\\ u(x,0)=0, & x\in\Omega, \end{cases} \tag{1.2}$$

where $T>0$ is a fixed final time, $u_d:(0,T)\to L^2(\Omega)$ is a given target function, $\gamma>0$ is a penalty constant, and q is the unknown control variable belonging to the admissible set U_{ad} given by

$$U_{ad} = \left\{q\in L^2(0,T;L^2(\Omega)) : a\leq q\leq b \ \text{ a.e. in } \Omega\times[0,T]\right\}, \tag{1.3}$$

with $a,b\in\mathbb{R}$ and $a\leq b$. In (1.2), $D_t^{1-\alpha,x}$ with $\alpha\in(0,1)$ represents the left-sided Riemann-Liouville fractional substantial derivative [2, 7, 18] as follows:

$$D_t^{1-\alpha,x}u(x,t) = \frac{1}{\Gamma(\alpha)}\left[\partial_t+\rho U(x)\right]\int_0^t (t-s)^{\alpha-1}e^{-(t-s)\rho U(x)}u(x,s)ds, \tag{1.4}$$

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where $\Gamma(s) = \int_0^\infty t^{s-1}e^{-t}dt$ is the Euler-gamma function, $\rho \in \mathbb{C}$, Δ denotes the Laplace operator, the function $U(x)$ is given and bounded in $\bar{\Omega}$, and $f : (0,T) \to L^2(\Omega)$ is a given function. It is noticed that $D_t^{1-\alpha,x}\Delta \neq \Delta D_t^{1-\alpha,x}$ if $\rho U(x)$ is not a constant function.

The backward fractional Feynman-Kac equation (1.2) was derived by Carmi et al. in [2, 34] to depict the probability density function of a functional of non-Brownian motion with power-law waiting time, which is a widespread phenomenon in various multiscale fields, including physics, chemistry, biology, finance and others [9, 22, 23, 27, 28, 29, 36]. Specifically, (1.2) is the governing equation of $u(x,\rho,t) := \int_0^\infty u(x,\mathbb{A},t)e^{-\rho\mathbb{A}}d\mathbb{A}$, where $\mathbb{A} = \int_0^t U(x(s))ds$ is the functional of anomalous diffusion in non-Brownian motion with $U(x)$ being a prescribed nonnegative function associated with specific applications [2, 4], and $u(x,\mathbb{A},t)$ denotes the probability density function of finding the particle's path functional on $\mathbb{A}$ at the time t with the initial position of the particle at x. A variant equation of (1.2) is obtained replacing ρ by $-\mathbf{i}\rho$ [2] if the functional $\mathbb{A}$ is not definitely nonnegative induced by some non-positive function $U(x)$, and it is the governing equation of the Fourier transform of $u(x,\mathbb{A},t)$, i.e., $u(x,\rho,t) := \int_{-\infty}^{+\infty} u(x,\mathbb{A},t)e^{\mathbf{i}\rho\mathbb{A}}\mathrm{d}\mathbb{A}$ with $\mathbf{i}$ being the imaginary unit. Another variant of (1.2), named the forward fractional Feynman-Kac equation, is as follows:

$$\partial_t u(x,t) - \Delta D_t^{1-\alpha,x}u(x,t) + \rho U(x)u(x,t) = f(x,t) + q(x,t) \tag{1.5}$$

with the term $D_t^{1-\alpha,x}\Delta u$ in (1.2) being replaced by $\Delta D_t^{1-\alpha,x}u$, it describes the joint probability density function of finding the particle on $(x,\mathbb{A})$ at time t. It is essentially different from (1.2) due to the noncommutativity of the nonlocal operator $D_t^{1-\alpha,x}$ defined by (1.4) and the Laplacian Δ whenever $\rho U(x)$ is not a constant function.

Equation (1.2) covers many important models. If $\alpha = 1$, it leads to the classical Feynman-Kac equation describing the functional distribution of Brownian motion, which is a Schrödinger-like equation derived by Kac [16] in 1949 by using the Feynman's path integral method. If $\rho U(x) \equiv 0$ and $\alpha \in (0,1)$, then (1.2) becomes the time-fractional diffusion equation $\partial_t u - D_t^{1-\alpha}\Delta u = 0$ as $D_t^{1-\alpha,x}$ in (1.2) deduces to the Riemann-Liouville fractional derivative $D_t^{1-\alpha}$ defined by (2.7), and it describes many anomalous diffusion phenomena in physics, chemistry, biology, finance and others [22, 23, 36].

A number of efficient numerical algorithms have been designed for solving time-fractional partial differential equations, but the numerical investigations of the fractional Feynman-Kac equations are relatively limited. Due to the time-space coupled nonlocal operator $D_t^{1-\alpha,x}$ in (1.4) and its noncommutativity with the Laplacian Δ in the equations, it encounters significant challenges on numerical discretizations and their error analyses. Chen and Deng [3] established high-order finite difference approximations for fractional substantial derivatives based on the Lubich method [21], which were subsequently used to numerically solve the forward and backward fractional Feynman-Kac equations with smooth solutions [5]. Recently, Sun, Nie and Deng [30] concerned the first-order and second-order time-stepping schemes for the homogeneous backward fractional Feynman-Kac equation with nonsmooth initial data by using the convolution quadrature approximations of the fractional substantial derivative. Later, high-order fully discrete schemes with some correction terms were developed for the backward fractional Feynman-Kac equation by combining the backward difference formulas (BDF) convolution quadrature in time and the finite element method in space [31]. In [13], the authors proposed and analyzed a second-order time-stepping numerical scheme for the inhomogeneous backward fractional Feynman-Kac equation with nonsmooth initial data by using the weighted and shifted Grünwald difference (WSGD) formula [33]. A first-order time-stepping method was provided in [6] to solve the forward fractional Feynman-Kac equation with error estimates in the measure norm depending only on the measure of the initial data. The work [25] considered the forward fractional Feynman-Kac equation, built the regularity of the solution, and developed the error estimates for a fully discrete scheme constructed by convolution quadrature and finite element methods.

Substantial researches have emerged over the past decade discussing optimal control problems of fractional partial differential equations, addressing both theoretical and numerical issues, one can consult the works [1, 12, 15, 20, 24, 35, 37, 38] and the references therein. Despite all this, the optimal control problem of the backward fractional Feynman-Kac equation has not yet been explored. In our recent work [14], an optimal control problem of the forward fractional Feynman-Kac equation (1.5) was discussed, which is essentially different from the problem (1.1)-(1.2) due to the difference of their constrained state equations (1.5) and (1.2) as mentioned before, and thus the results do not apply to (1.1)-(1.2). To fill this gap, we endeavor to investigate the theoretic and numerical analysis of the optimal control problem (1.1)-(1.2), where the complex parameter ρ and the noncommutativity of the time-space coupled nonlocal operator $D_t^{1-\alpha,x}$ and the Laplacian Δ pose noteworthy challenges. We will first derive the first-order optimality conditions and analyze the solution's regularity. Then we propose and rigorously analyze a temporal semidiscrete scheme for the optimal control problem, which is proved to exhibit an almost optimal convergence order of $O(\tau|\ln\tau|)$ in time relying solely on regularity assumptions of the data without the regularity requirements on the exact solution.

The rest of this paper is organized as follows. In Section 2, we derive the optimality conditions and the solution representations, and establish the regularity results of the solution to the optimal control problem (1.1)-(1.2). In Section 3, a first order temporal semidiscrete scheme is proposed for solving (1.1)-(1.2) with the Riemann-Liouville fractional substantial derivative in time approximated by the backward Euler convolution quadrature (BECQ) formula. In Section 4, we rigorously analyze the temporal error estimates of the proposed semidiscrete scheme. The theoretical convergence result of our proposed numerical scheme is verified by numerical examples in Section 5. This paper ends with some conclusions in Section 6.

2. The continuous optimal control problem.

In this section, we discuss the well-posedness and the first-order optimality conditions of the continuous optimal control problem (1.1)-(1.2), derive the solution representations and estimate their regularity results.

2.1. Optimality conditions and solution representations.

THEOREM 2.1. *The optimal control problem (1.1)-(1.2) has a unique solution (u,q) in $L^2(0,T;L^2(\Omega))\times U_{ad}$. In addition, there exists an adjoint state $z\in L^2(0,T;L^2(\Omega))$ such that (u,z,q) satisfies the optimality conditions*

$$\begin{cases}\partial_t u - D_t^{1-\alpha,x}\Delta u + \rho U(x)u = f+q, & (x,t)\in\Omega\times(0,T],\\ u(x,t)=0, & (x,t)\in\partial\Omega\times(0,T],\\ u(x,0)=0, & x\in\Omega,\end{cases} \tag{2.1}$$

$$
\begin{cases} -\partial_t z - \Delta {}^B D_t^{1-\alpha,x} z + \rho U(x) z = u - u_d, & (x,t) \in \Omega \times (0,T], \\ z(x,t) = 0, & (x,t) \in \partial\Omega \times (0,T], \\ z(x,T) = 0, & x \in \Omega, \end{cases} \tag{2.2}
$$

and the variational inequality

$$
J'(q)(v-q) = \int_0^T \int_\Omega (\gamma q + z)(v-q) \mathrm{d}x\mathrm{d}t \geq 0 \quad \forall\ v \in U_{ad}, \tag{2.3}
$$

where ${}^B D_t^{1-\alpha,x}$ *is the adjoint operator of* $D_t^{1-\alpha,x}$*, and called the right-sided Riemann-Liouville fractional substantial derivative given by*

$$
{}^B D_t^{1-\alpha,x} z(x,t) = e^{t\rho U(x)} {}^B D_t^{1-\alpha} \big(e^{-t\rho U(x)} z(x,t) \big), \tag{2.4}
$$

with ${}^B D_t^{1-\alpha}$ *being the right-sided Riemann-Liouville fractional derivative [26] defined by*

$$
{}^B D_t^{1-\alpha} z(x,t) = -\frac{1}{\Gamma(\alpha)} \partial_t \int_t^T (s-t)^{\alpha-1} z(x,s) \mathrm{d}s, \quad \alpha \in (0,1).
$$

Proof. Let q be a minimizer of $J(q) := J(u(q), q)$, and $\delta u(q) := \lim_{\epsilon \to 0} [u(q + \epsilon(v - q)) - u(q)]/\epsilon$, it yields from (1.2) that $\delta u(q)$ satisfies

$$
\partial_t \delta u(q) - D_t^{1-\alpha,x} \Delta \delta u(q) + \rho U(x) \delta u(q) = v - q \tag{2.5}
$$

with zero boundary and initial values. Then we easily have the first-order necessary optimality condition of the optimal control problem (1.1)-(1.2) as follows:

$$
J'(q)(v-q) = \int_0^T \int_\Omega (u - u_d) \delta u(q) \mathrm{d}x\mathrm{d}t + \int_0^T \int_\Omega \gamma q (v-q) \mathrm{d}x\mathrm{d}t \geq 0 \quad \forall\ v \in U_{ad}.
$$

The fractional substantial derivative (1.4) satisfies (see [18])

$$
D_t^{1-\alpha,x} u(x,t) = e^{-t\rho U(x)} D_t^{1-\alpha} \big(e^{t\rho U(x)} u(x,t) \big), \tag{2.6}
$$

where $D_t^{1-\alpha}$ refers to the left-sided Riemann-Liouville fractional derivative [26] given by

$$
D_t^{1-\alpha} u(x,t) = \frac{1}{\Gamma(\alpha)} \partial_t \int_0^t (t-s)^{\alpha-1} u(x,s) ds, \quad \alpha \in (0,1). \tag{2.7}
$$

Subsequently, by the fractional integration by parts formula of the left- and right-sided Riemann-Liouville fractional derivatives in [19, Lemma 2.3], it follows that

$$
\begin{aligned}
\int_0^T \int_\Omega \delta u(q) \cdot \Delta {}^B D_t^{1-\alpha,x} z \mathrm{d}x\mathrm{d}t &= \int_0^T \int_\Omega e^{t\rho U(x)} \Delta \delta u(q) \cdot {}^B D_t^{1-\alpha} \big(e^{-t\rho U(x)} z \big) \mathrm{d}x\mathrm{d}t \\
&= \int_0^T \int_\Omega e^{-t\rho U(x)} D_t^{1-\alpha} \big(e^{t\rho U(x)} \Delta \delta u(q) \big) \cdot z \mathrm{d}x\mathrm{d}t \\
&= \int_0^T \int_\Omega D_t^{1-\alpha,x} \Delta \delta u(q) \cdot z \mathrm{d}x\mathrm{d}t.
\end{aligned}
$$

Together with the above property, (2.2) and (2.5) with zero boundary and initial values, we derive

$$\begin{aligned}\int_0^T\int_\Omega (u-u_d)\delta u(q)\mathrm{d}x\mathrm{d}t &= \int_0^T\int_\Omega \big(-\partial_t z - \Delta^B D_t^{1-\alpha,x} z + \rho U(x) z\big)\delta u(q)\mathrm{d}x\mathrm{d}t\\ &= \int_0^T\int_\Omega z\big(\partial_t \delta u(q) - D_t^{1-\alpha,x}\Delta\delta u(q) + \rho U(x)\delta u(q)\big)\mathrm{d}x\mathrm{d}t\\ &= \int_0^T\int_\Omega z(v-q)\mathrm{d}x\mathrm{d}t,\end{aligned}$$

which leads to the variational inequality (2.3).

Furthermore, we can easily deduce from (2.3) that the objective functional $J(\cdot)$ in (1.1) is strongly convex with respect to the control variable q, and

$$J'(p)(p-q) - J'(q)(p-q) \ge \gamma\|p-q\|^2_{L^2(0,T;L^2(\Omega))} \tag{2.8}$$

for any $p, q \in L^2(0,T;L^2(\Omega))$, which indicates the uniqueness of the solution to the continuous optimal control problem (1.1)-(1.2). □

It follows from the variational inequality (2.3) that

$$q = P_{U_{ad}}\Big(-\frac{1}{\gamma}z\Big), \tag{2.9}$$

where $P_{U_{ad}}(\cdot)$ is the pointwise projection onto the admissible set U_{ad}, given by

$$P_{U_{ad}}\big(v(t)\big) = \max\big\{a, \min\{v(t), b\}\big\}, \tag{2.10}$$

which has the following property [17, Corollary 2.4]:

$$\|P_{U_{ad}}(v)\|_{H^1(0,T;L^2(\Omega))} \le \|v\|_{H^1(0,T;L^2(\Omega))} + C \quad \forall\, v \in H^1(0,T;L^2(\Omega)). \tag{2.11}$$

Next, we derive the integral representations of the solutions to the state and adjoint equations (2.1) and (2.2). It yields from [18, Proposition 7] that the Laplace transform of the left-sided Riemann-Liouville fractional substantial derivative $D_t^{1-\alpha,x}$ in (1.4) with $\alpha \in (0,1)$ is

$$\mathcal{L}(D_t^{1-\alpha,x}u)(\xi) = \beta(\xi)^{1-\alpha}\hat{u}(\xi), \tag{2.12}$$

for $u(x,0)=0$, where $\mathcal{L}$ and $\hat{}$ both stand for the Laplace transform and

$$\beta(\xi) := \xi + \rho U(x). \tag{2.13}$$

Then we take the Laplace transform of (2.1) and obtain

$$\hat{u}(\xi) = \big(\beta(\xi)^\alpha - \Delta\big)^{-1}\beta(\xi)^{\alpha-1}\big(\hat{f}(\xi) + \hat{q}(\xi)\big). \tag{2.14}$$

By the rule of inverse Laplace transform $\mathcal{L}^{-1}(\hat{f}\hat{g})(t) = \int_0^t \mathcal{L}^{-1}(\hat{f})(t-s)\mathcal{L}^{-1}(\hat{g})(s)\mathrm{d}s$ and Cauchy's integral formula and theorem, it obtains the solution to (2.1) as follows:

$$u(\cdot,t) = \int_0^t F(t-s)\big(f(\cdot,s) + q(\cdot,s)\big)\mathrm{d}s, \tag{2.15}$$

where the operator $F(\cdot): L^2(\Omega) \to L^2(\Omega)$ is given by

$$F(t) := \frac{1}{2\pi \mathbf{i}} \int_{\Gamma_{\theta,\kappa}} e^{\xi t} \big(\beta(\xi)^\alpha - \Delta\big)^{-1} \beta(\xi)^{\alpha-1} \mathrm{d}\xi, \tag{2.16}$$

with $\beta(\xi)$ given by (2.13) and $\Gamma_{\theta,\kappa}$ defined as

$$\Gamma_{\theta,\kappa} = \big\{z \in \mathbb{C} : |z| = \kappa, |\arg z| \le \theta\big\} \cup \big\{z \in \mathbb{C} : |z| \ge \kappa,\ |\arg z| = \theta\big\}. \tag{2.17}$$

By the approach of the Laplace transform, we can also obtain the solution to (2.2) represented by

$$z(\cdot,t) = \int_t^T E(s-t)\big(u(\cdot,s) - u_d(\cdot,s)\big)\mathrm{d}s, \tag{2.18}$$

where the operator $E(\cdot): L^2(\Omega) \to L^2(\Omega)$ is given by

$$E(t) := \frac{1}{2\pi \mathbf{i}} \int_{\Gamma_{\theta,\kappa}} e^{\xi t} \beta(\xi)^{\alpha-1} \big(\beta(\xi)^\alpha - \Delta\big)^{-1} \mathrm{d}\xi. \tag{2.19}$$

If $\rho U(x)$ is not a constant function, then it is clear that $\beta(\xi)^{\alpha-1} \cdot \big(\beta(\xi)^\alpha - \Delta\big)^{-1} \neq \big(\beta(\xi)^\alpha - \Delta\big)^{-1} \cdot \beta(\xi)^{\alpha-1}$ due to (2.13), which indicates that the operators $F(\cdot)$ and $E(\cdot)$ are essentially different.

2.2. Solutions regularity. In this subsection, we establish the regularity results of the solution to the optimality system (2.1)-(2.3). First, we introduce two essential lemmas for further analysis. Throughout, the notation $\|\cdot\|$ denotes the operator norm from $L^2(\Omega)$ to $L^2(\Omega)$.

LEMMA 2.2 ([10]). *For $\xi \in \Sigma_\theta := \big\{\xi \in \mathbb{C}\backslash\{0\} : |\arg \xi| \le \theta\big\}$ with $\theta \in (0,\pi)$, we have the resolvent estimates*

$$\|(\xi - \Delta)^{-1}\| \le C|\xi|^{-1}, \tag{2.20}$$

$$\|\Delta^{1-\gamma}(\xi - \Delta)^{-1}\| \le C|\xi|^{-\gamma},\ \gamma \in [0,1]. \tag{2.21}$$

LEMMA 2.3 ([6, 30]). *Let $\beta(\xi)$ be defined in (2.13) and $U(x)$ bounded in $\bar{\Omega}$. By choosing $\theta \in (\frac{\pi}{2}, \pi)$ sufficiently close to $\frac{\pi}{2}$ and $\kappa > 0$ sufficiently large (depending on $|\rho|\|U(x)\|_{L^\infty(\bar{\Omega})}$), we have the following results.*

(1) For all $x \in \Omega$ and $\xi \in \Sigma_{\theta,\kappa}$, it holds that $\beta(\xi) \in \Sigma_{\frac{3\pi}{4},\frac{\kappa}{2}}$ and

$$C_1|\xi| \le |\beta(\xi)| \le C_2|\xi|,$$

where C_1, C_2 are positive constants. Thus $\beta(\xi)^{1-\alpha}$ and $\beta(\xi)^{\alpha-1}$ are both $C(\bar{\Omega})$ valued analytic function of $\xi \in \Sigma_{\theta,\kappa} := \big\{z \in \mathbb{C} : |z| \ge \kappa, |\arg z| \le \theta\big\}$.

(2) The operator $(\beta(\xi)^\alpha - \Delta)^{-1} : L^2(\Omega) \to L^2(\Omega)$ is well-defined, bounded, and analytic for $z \in \Sigma_{\theta,\kappa}$, satisfying

$$\|(\beta(\xi)^\alpha - \Delta)^{-1}\| \le C|\xi|^{-\alpha} \quad \forall\ \xi \in \Sigma_{\theta,\kappa},$$
$$\|\Delta(\beta(\xi)^\alpha - \Delta)^{-1}\| \le C \quad \forall\ \xi \in \Sigma_{\theta,\kappa}.$$

The regularity results of the solutions to the optimality conditions (2.1)-(2.3) are provided in the following theorem.

THEOREM 2.4. *Let $f, u_d \in L^2(0,T;L^2(\Omega))$, $U(x) \in W^{2,\infty}(\Omega)$ and the real part $\mathrm{Re}(\rho U(x)) \geq 0$. Then the solutions (u, z, q) to the system (2.1)-(2.3) satisfy*

$$\|u\|_{H^1(0,T;L^2(\Omega))} + \|u\|_{L^2(0,T;\dot{H}^2(\Omega))} \leq C\|f+q\|_{L^2(0,T;L^2(\Omega))}, \tag{2.22}$$

$$\|z\|_{H^1(0,T;L^2(\Omega))} + \|z\|_{L^2(0,T;\dot{H}^2(\Omega))} \leq C\left\|u-u_d\right\|_{L^2(0,T;L^2(\Omega))}, \tag{2.23}$$

$$\|q\|_{H^1(0,T;L^2(\Omega))} \leq C\left\|u-u_d\right\|_{L^2(0,T;L^2(\Omega))} + C, \tag{2.24}$$

where $\dot{H}^2(\Omega) = H^2(\Omega) \cap H_0^1(\Omega)$ equipped with the norm $\|v\|_{\dot{H}^2(\Omega)} = \|\Delta v\|_{L^2(\Omega)}$.

Proof. For the operator $F(t)$ in (2.16), it follows from Lemma 2.3 that

$$\|F(t)\| \leq C \quad \text{and} \quad \|\Delta F(t)\| \leq Ct^{-\alpha}. \tag{2.25}$$

Then the representation of u in (2.15) directly implies that

$$\|u(t)\|_{L^2(\Omega)} \leq C\int_0^t \|(f+q)(s)\|_{L^2(\Omega)}\mathrm{d}s,$$
$$\|u(t)\|_{\dot{H}^2(\Omega)} \leq C\int_0^t (t-s)^{-\alpha}\|(f+q)(s)\|_{L^2(\Omega)}\mathrm{d}s,$$

which leads to the following estimates by Young's inequality for convolution that

$$\|u\|_{L^2(0,T;L^2(\Omega))} + \|u\|_{L^2(0,T;\dot{H}^2(\Omega))} \leq C\|f+q\|_{L^2(0,T;L^2(\Omega))}. \tag{2.26}$$

By extending u to be zero for $t<0$ and f, q to be zero for $t \in \mathbb{R}\backslash[0,T]$, it derives from (2.14) that

$$\begin{aligned}(\partial_t + \rho U(x))u &= \mathcal{L}^{-1}\big\{\beta(\xi)\mathcal{L}u(\xi)\big\}(t)\\ &= \mathcal{F}^{-1}\big\{\beta(\mathbf{i}\omega)\big(\beta(\mathbf{i}\omega)^\alpha - \Delta\big)^{-1}\beta(\mathbf{i}\omega)^{\alpha-1}\mathcal{F}(f+q)(\omega)\big\}(t),\end{aligned}$$

where it applies $\mathcal{F}v(\omega) = \mathcal{L}v(\xi)$ with $\xi = \mathbf{i}\omega$ and $\omega \in \mathbb{R}$, and $\mathcal{F}$ refers to the Fourier transform. It also holds that $\beta(\mathbf{i}\omega) \in \Sigma_{\frac{\pi}{2}}$ due to $\mathrm{Re}(\rho U(x)) \geq 0$. Then, by Lemma 2.2 and the Plancherel formula, we have that

$$\begin{aligned}&\|(\partial_t + \rho U(x))u\|_{L^2(0,T;L^2(\Omega))} \leq \|(\partial_t + \rho U(x))u\|_{L^2(\mathbb{R};L^2(\Omega))}\\ &= \|\mathcal{F}^{-1}\big\{\beta(\mathbf{i}\omega)\big(\beta(\mathbf{i}\omega)^\alpha - \Delta\big)^{-1}\beta(\mathbf{i}\omega)^{\alpha-1}\mathcal{F}(f+q)\big\}\|_{L^2(\mathbb{R};L^2(\Omega))}\\ &= \|\beta(\mathbf{i}\omega)\big(\beta(\mathbf{i}\omega)^\alpha - \Delta\big)^{-1}\beta(\mathbf{i}\omega)^{\alpha-1}\mathcal{F}(f+q)\|_{L^2(\mathbb{R};L^2(\Omega))}\\ &\leq C\|\mathcal{F}(f+q)\|_{L^2(\mathbb{R};L^2(\Omega))} = C\|f+q\|_{L^2(\mathbb{R};L^2(\Omega))}\\ &= C\|f+q\|_{L^2(0,T;L^2(\Omega))},\end{aligned}$$

which and $U(x) \in L^\infty(\Omega)$ imply

$$\|\partial_t u\|_{L^2(0,T;L^2(\Omega))} \leq C\|f+q\|_{L^2(0,T;L^2(\Omega))}. \tag{2.27}$$

Thus, (2.26) and (2.27) lead to the estimate (2.22).

Next, we consider to obtain the estimate (2.23). With some calculations, we have

$$\nabla\beta(\xi)^{\alpha-1} = (\alpha-1)\rho\beta(\xi)^{\alpha-2}\nabla U(x),$$
$$\Delta\beta(\xi)^{\alpha-1} = (\alpha-1)\rho\big(\rho(\alpha-2)\beta(\xi)^{\alpha-3}\nabla U(x)\cdot\nabla U(x) + \beta(\xi)^{\alpha-2}\Delta U(x)\big).$$

Together with the condition $U(x) \in W^{2,\infty}(\Omega)$, Lemma 2.3, the equivalence of the norms $\|\cdot\|_{\dot H^2(\Omega)}$ and $\|\cdot\|_{H^2(\Omega)}$ in $\dot H^2(\Omega)$ (see [32, Lemma 3.1]), then it derives that $\|\nabla\beta(\xi)^{\alpha-1}\|_{L^\infty(\Omega)} + \|\Delta\beta(\xi)^{\alpha-1}\|_{L^\infty(\Omega)} \le C|\xi|^{\alpha-1}$ for any $\xi \in \Gamma_{\theta,\kappa}$, and

$$\begin{aligned}\|\beta(\xi)^{\alpha-1}v\|_{\dot H^2(\Omega)} &= \|\Delta(\beta(\xi)^{\alpha-1}v)\|_{L^2(\Omega)}\\ &\le \|(\Delta\beta(\xi)^{\alpha-1})v\|_{L^2(\Omega)} + 2\|\nabla\beta(\xi)^{\alpha-1}\cdot\nabla v\|_{L^2(\Omega)}\\ &\quad + \|\beta(\xi)^{\alpha-1}\Delta v\|_{L^2(\Omega)}\\ &\le C|\xi|^{\alpha-1}\|v\|_{\dot H^2(\Omega)} \quad \forall\, \xi \in \Gamma_{\theta,\kappa},\end{aligned}$$

where $|\xi| \ge \kappa$ is applied. Then it further derives from (2.19) and Lemma 2.3 that $\|E(t)\| \le C$ and

$$\begin{aligned}\|\Delta E(t)\| &\le C\int_{\Gamma_{\theta,\kappa}} |e^{\xi t}|\|\beta(\xi)^{\alpha-1}\|_{\dot H^2(\Omega)\to\dot H^2(\Omega)}\|\big(\beta(\xi)^\alpha - \Delta\big)^{-1}\|_{L^2(\Omega)\to\dot H^2(\Omega)}|\mathrm{d}\xi|\\ &\le C\int_{\Gamma_{\theta,\kappa}} |e^{\xi t}|\cdot|\xi|^{\alpha-1}|\mathrm{d}\xi| \le Ct^{-\alpha},\end{aligned}$$

which implies from (2.18) that

$$\|z\|_{L^2(0,T;L^2(\Omega))} + \|z\|_{L^2(0,T;\dot H^2(\Omega))} \le C\|u-u_d\|_{L^2(0,T;L^2(\Omega))}. \tag{2.28}$$

To obtain the estimate $\|\partial_t z\|_{L^2(0,T;L^2(\Omega))}$, we let $p(\cdot,\eta) := z(\cdot, T-\eta)$ with $\eta = T-t$ given by

$$p(\eta) = \int_0^\eta E(\eta - r)(\bar u - \bar u_d)(r)\mathrm{d}r, \tag{2.29}$$

which satisfies the following equation

$$\partial_\eta p(\eta) - \Delta D_\eta^{1-\alpha,x} p(\eta) + \rho U(x)p(\eta) = (\bar u - \bar u_d)(\eta), \quad \eta \in (0,T], \quad \text{with} \quad p(0) = 0,$$

where $\bar u(\cdot,\eta) = u(\cdot, T-\eta)$ and $\bar u_d(\cdot,\eta) = u_d(\cdot, T-\eta)$. Then by the similar approach for (2.27), we can derive (2.23). Finally, (2.9) and (2.11) lead to the estimate (2.24).□

3. Discretization in time.

In this section, a temporal semidiscrete scheme is designed for solving the optimal control problem (1.1)-(1.2) governed by the backward fractional Feymann-Kac equation, then the corresponding optimality conditions and the representations of the discrete solutions are established.

3.1. A semidiscrete scheme.

Let $t_n = n\tau$ $(n = 0, 1, \ldots, N)$ be the isometric points in the time interval $[0,T]$ with the step size $\tau = T/N$. We discretize the optimal control problem (1.1)-(1.2) in the time direction as follows:

$$\min_{\mathbf{Q}\in U_{ad}^\tau} J(\mathbf{Q}) = \frac{\tau}{2}\sum_{n=1}^N \left(\|U^n - u_d^n\|^2_{L^2(\Omega)} + \gamma\|Q^{n-1}\|^2_{L^2(\Omega)}\right) \tag{3.1}$$

subject to

$$\begin{cases} \bar D_\tau^{1,x} U^n - \bar D_\tau^{1-\alpha,x}\Delta U^n = f^n + Q^{n-1}, & x \in \Omega, \quad n = 1, 2, \ldots, N,\\ U^n = 0, & x \in \partial\Omega, \quad n = 0, 1, \ldots, N,\\ U^0 = 0, & x \in \Omega, \end{cases} \tag{3.2}$$

where $f^n = \frac{1}{\tau}\int_{t_{n-1}}^{t_n} f(\cdot,t)\mathrm{d}t$, $u_d^n = \frac{1}{\tau}\int_{t_{n-1}}^{t_n} u_d(\cdot,t)\mathrm{d}t$, and

$$U_{ad}^{\tau} = \left\{\mathbf{Q} = \left(Q^{n-1}\right)_{n=1}^{N} : a \le Q^{n-1} \le b,\ n = 1,2,\dots,N\right\}.$$

In (3.2), the difference operator $\bar{D}_{\tau}^{1-\alpha,x}$ is given by

$$\bar{D}_{\tau}^{1-\alpha,x} U^n := \frac{1}{\tau^{1-\alpha}} \sum_{j=1}^{n} b_{n-j}^{(1-\alpha)} e^{-t_{n-j}\rho U(x)} U^j, \quad n = 1,2,\dots,N, \tag{3.3}$$

to approximate the Riemann-Liouville fractional substantial derivative $D_t^{1-\alpha,x}u(x,t_n)$ in the state equation (1.2), see [3, 6, 30]. The coefficients $\{b_j^{(1-\alpha)}\}$ in (3.3) satisfy the power series expansion

$$\big(\delta_\tau(\zeta)\big)^{1-\alpha} = \frac{1}{\tau^{1-\alpha}} \sum_{j=0}^{\infty} b_j^{(1-\alpha)} \zeta^j \quad \forall\, |\zeta| < 1, \quad \text{with} \quad \delta_\tau(\zeta) = \frac{1-\zeta}{\tau}, \tag{3.4}$$

and can be evaluated by the recursive formula $b_0^{(1-\alpha)} = 1,\ b_j^{(1-\alpha)} = b_{j-1}^{(1-\alpha)} \cdot \frac{\alpha+j-2}{j},\ j = 1,2,\dots$. In addition, $\bar{D}_\tau^{1,x} U^n$ refers to

$$\bar{D}_\tau^{1,x} U^n := e^{-t_n \rho U(x)} \bar{D}_\tau (e^{t_n \rho U(x)} U^n) = \frac{U^n - e^{-\tau\rho U(x)} U^{n-1}}{\tau}, \tag{3.5}$$

for discretizing the terms $\partial_t u + \rho U(x) u$ due to the relationship $\partial_t u + \rho U(x) u = e^{-t\rho U(x)} \partial_t (e^{t\rho U(x)} u)$, and $\bar{D}_\tau$ represents the standard backward Euler difference operator $\bar{D}_\tau U^n := \frac{U^n - U^{n-1}}{\tau}$.

Moreover, we denote ${}^{B}\bar{D}_\tau Z^{n-1} := \frac{Z^{n-1} - Z^n}{\tau}$, and introduce the adjoint difference operators of those in (3.3) and (3.5), as follows:

$${}^{B}\bar{D}_{\tau}^{1-\alpha,x} Z^{n-1} := \frac{1}{\tau^{1-\alpha}} \sum_{j=n}^{N} b_{j-n}^{(1-\alpha)} e^{-t_{j-n}\rho U(x)} Z^{j-1}, \tag{3.6}$$

$${}^{B}\bar{D}_{\tau}^{1,x} Z^{n-1} := e^{t_{n-1}\rho U(x)}\, {}^{B}\bar{D}_\tau (e^{-t_{n-1}\rho U(x)} Z^{n-1}) = \frac{Z^{n-1} - e^{-\tau\rho U(x)} Z^n}{\tau}, \tag{3.7}$$

which are the temporal difference approximations of ${}^{B}D_t^{1-\alpha,x} z(x,t_{n-1})$ and $(-\partial_t + \rho U(x)) z(x,t_{n-1})$ in the adjoint equation (2.2), respectively. Then we have the following relationships:

$$\tau \sum_{n=1}^{N} ({}^{B}\bar{D}_{\tau}^{1-\alpha,x} Z^{n-1}, U^n) = \tau \sum_{n=1}^{N} (Z^{n-1}, \bar{D}_{\tau}^{1-\alpha,x} U^n), \tag{3.8}$$

$$\tau \sum_{n=1}^{N} ({}^{B}\bar{D}_{\tau}^{1,x} Z^{n-1}, U^n) = \tau \sum_{n=1}^{N} (Z^{n-1}, \bar{D}_{\tau}^{1,x} U^n), \tag{3.9}$$

where $U^0 = 0$ and $Z^N = 0$.

3.2. Optimality conditions and solution representations. As the functional $J(\cdot)$ in (3.1) is strongly convex, then the temporal semidiscrete problem (3.1)-(3.2) has a unique solution $(\mathbf{U}, \mathbf{Q})$. By (3.8), (3.9), and the similar approach as in the proof of Theorem 2.1, we can obtain that there exists an adjoint state $\mathbf{Z}$ such that $(\mathbf{U}, \mathbf{Z}, \mathbf{Q})$ satisfies the optimality system

$$\bar{D}_\tau^{1,x} U^n - \bar{D}_\tau^{1-\alpha,x} \Delta U^n = f^n + Q^{n-1}, \qquad x \in \Omega, \quad U^n = 0, \; x \in \partial\Omega, \tag{3.10}$$

$$^B\bar{D}_\tau^{1,x} Z^{n-1} - \Delta {}^B\bar{D}_\tau^{1-\alpha,x} Z^{n-1} = U^n - u_d^n, \quad x \in \Omega, \quad Z^{n-1} = 0, \; x \in \partial\Omega, \tag{3.11}$$

for $n = 1, 2, \ldots, N$ with $U^0 = 0$, $Z^N = 0$, and the variational inequality

$$(\gamma Q^{n-1} + Z^{n-1}, v - Q^{n-1}) \geq 0 \quad \forall\, v \in L^2(\Omega), \; a \leq v \leq b, \tag{3.12}$$

where

$$\mathbf{U} = (U^n)_{n=1}^N, \quad \mathbf{Z} = (Z^{n-1})_{n=1}^N, \quad \mathbf{Q} = (Q^{n-1})_{n=1}^N. \tag{3.13}$$

To derive the solution representations for the temporal semidiscrete schemes (3.10)-(3.11), we first introduce the functions as follows:

$$f_\tau(\cdot, t)|_{(t_{n-1}, t_n]} = f^n, \quad Q(\cdot, t)|_{[t_{n-1}, t_n)} = Q^{n-1}, \quad n = 1, 2, \ldots, N, \tag{3.14}$$

$$U(\cdot, t)|_{(t_{n-1}, t_n]} = U^n, \quad u_{d\tau}(\cdot, t)|_{(t_{n-1}, t_n]} = u_d^n, \quad n = 1, 2, \ldots, N. \tag{3.15}$$

Let $\tilde{U}(\zeta) = \sum_{n=1}^\infty U^n \zeta^n$, it obtains from (3.3), (3.4) and (3.5) that

$$\sum_{n=1}^\infty (\bar{D}_\tau^{1-\alpha,x} U^n) \zeta^n = \delta_\tau(e^{-\tau\rho U(x)}\zeta)^{1-\alpha} \tilde{U}(\zeta),$$

$$\sum_{n=1}^\infty (\bar{D}_\tau^{1,x} U^n) \zeta^n = \delta_\tau(e^{-\tau\rho U(x)}\zeta) \tilde{U}(\zeta).$$

Then we multiply (3.10) by ζ^n and take the summation for n from 1 to ∞ that

$$\tilde{U}(\zeta) = \big(\delta_\tau(e^{-\tau\rho U(x)}\zeta)^\alpha - \Delta\big)^{-1} \delta_\tau(e^{-\tau\rho U(x)}\zeta)^{\alpha-1} \sum_{n=1}^\infty (f^n + Q^{n-1}) \zeta^n. \tag{3.16}$$

By using the following equality due to (3.14)

$$\hat{f}_\tau(\cdot, \xi) + \hat{Q}(\cdot, \xi) = \sum_{n=1}^\infty \int_{t_{n-1}}^{t_n} \big(f_\tau(\cdot, t) + Q(\cdot, t)\big) e^{-\xi t} \mathrm{d}t = \frac{e^{\xi\tau} - 1}{\xi} \sum_{n=1}^\infty (f^n + Q^{n-1}) e^{-\xi t_n},$$

we derive from (3.16), Cauchy's integral formula and theorem that the solution to (3.10) is represented by

$$U^n = \int_0^{t_n} F^\tau(t_n - s) \big(f_\tau(\cdot, s) + Q(\cdot, s)\big) \mathrm{d}s, \tag{3.17}$$

where

$$F^\tau(t) = \frac{1}{2\pi \mathbf{i}} \int_{\Gamma_{\theta,\kappa}^\tau} e^{\xi t} \frac{\xi\tau}{e^{\xi\tau} - 1} \big(\delta_\tau(e^{-\tau\beta(\xi)})^\alpha - \Delta\big)^{-1} \delta_\tau(e^{-\tau\beta(\xi)})^{\alpha-1} \mathrm{d}\xi, \tag{3.18}$$

and $\Gamma_{\theta,\kappa}^\tau$ is given by

$$\Gamma_{\theta,\kappa}^\tau = \Big\{z \in \mathbb{C} : |z| = \kappa, \; |\arg z| \leq \theta\Big\} \cup \Big\{z \in \mathbb{C} : \kappa \leq |z| \leq \frac{\pi}{\tau \sin\theta}, \; |\arg z| = \theta\Big\}.$$

Similarly, we can obtain the solution representation of (3.11) as follows:

$$Z^{n-1} = \int_{t_{n-1}}^{T} E^{\tau}(s - t_{n-1})\big(U(\cdot,s) - u_{d\tau}(\cdot,s)\big)\mathrm{d}s, \tag{3.19}$$

where

$$E^{\tau}(t) = \frac{1}{2\pi\mathbf{i}}\int_{\Gamma^{\tau}_{\theta,\kappa}} e^{\xi t}\frac{\xi\tau}{e^{\xi\tau}-1}\delta_{\tau}(e^{-\tau\beta(\xi)})^{\alpha-1}\big(\delta_{\tau}(e^{-\tau\beta(\xi)})^{\alpha} - \Delta\big)^{-1}\mathrm{d}\xi. \tag{3.20}$$

4. Stability and error estimates.

In this section, the error estimates of the proposed temporal semidiscrete scheme (3.1)-(3.2) are rigorously established in Theorem 4.7 without the regularity requirement on the solutions of the optimality system.

4.1. Stability.

In this subsection, we discuss the stability of the temporal semidiscrete scheme (3.1)-(3.2), which is crucial for the error estimates. A preliminary lemma as follows is first introduced for further analysis.

LEMMA 4.1 ([6, 30]). *Let $\beta(\xi)$ be given by (2.13) and $U(x)$ bounded in $\bar{\Omega}$. By choosing $\theta \in (\frac{\pi}{2}, \pi)$ sufficiently close to $\frac{\pi}{2}$ and $\kappa > 0$ sufficiently large (depending on $|\rho|\|U(x)\|_{L^{\infty}(\bar{\Omega})}$), there exists a positive constant τ_* such that the following estimates hold for $\tau \le \tau_*$.*

(1) For all $x \in \bar{\Omega}$ and $\xi \in \Sigma^{\tau}_{\theta,\kappa}$, we have $\delta_{\tau}(e^{-\tau\beta(\xi)}) \in \Sigma_{\frac{3\pi}{4},C_1\kappa}$ and

$$C_1|\xi| \le |\delta_{\tau}(e^{-\tau\beta(\xi)})| \le C_2|\xi|.$$

(2) The operator $(\delta_{\tau}(e^{-\tau\beta(\xi)})^{\alpha} - \Delta)^{-1} : L^2(\Omega) \to L^2(\Omega)$ is well-defined, bounded, and analytic with respect to $\xi \in \Sigma^{\tau}_{\theta,\kappa}$, satisfying

$$\begin{aligned}
&\|\Delta(\delta_{\tau}(e^{-\tau\beta(\xi)})^{\alpha} - \Delta)^{-1}\| \le C && \forall\ \xi \in \Sigma^{\tau}_{\theta,\kappa},\\
&\|(\delta_{\tau}(e^{-\tau\beta(\xi)})^{\alpha} - \Delta)^{-1}\| \le C|\xi|^{-\alpha} && \forall\ \xi \in \Sigma^{\tau}_{\theta,\kappa},
\end{aligned}$$

where $\Sigma^{\tau}_{\theta,\kappa} = \big\{\xi \in \mathbb{C} : |\xi| \ge \kappa,\ |\arg\xi| \le \theta,\ |\mathrm{Im}(\xi)| \le \frac{\pi}{\tau},\ \mathrm{Re}(\xi) \le \kappa+1\big\}$ with $\mathrm{Im}(\xi)$ and $\mathrm{Re}(\xi)$ being the imaginary and real parts of ξ, respectively.

(3) For all $x \in \bar{\Omega}$ and real number γ, it holds that

$$|\delta_{\tau}(e^{-\tau\beta(\xi)})^{\gamma} - \beta(\xi)^{\gamma}| \le C\tau|\xi|^{\gamma+1} \quad \forall\ \xi \in \Gamma^{\tau}_{\theta,\kappa}.$$

For further analysis, we utilize the discrete time-space inner product and norm defined as follows.

$$[\mathbf{v},\mathbf{w}] = \tau\sum_{n=1}^{N}(v^n, w^n) \quad \forall\ \mathbf{v} = (v^n)_{n=1}^{N}, \quad \mathbf{w} = (w^n)_{n=1}^{N} \in L^2(\Omega)^N,$$

$$|||\mathbf{v}||| = \sqrt{[\mathbf{v},\mathbf{v}]} = \Big(\tau\sum_{n=1}^{N}\|v^n\|^2_{L^2(\Omega)}\Big)^{\frac{1}{2}} \quad \forall\ \mathbf{v} = (v^n)_{n=1}^{N} \in L^2(\Omega)^N.$$

In addition, two auxiliary problems are introduced as follows for the error analysis of the temporal semidiscrete problem (3.1)-(3.2):

$$\begin{cases}
\bar{D}^{1,x}_{\tau}U(\mathbf{v})^n - \bar{D}^{1-\alpha,x}_{\tau}\Delta U(\mathbf{v})^n = f^n + v^{n-1}, & x \in \Omega, \quad n = 1,2,\dots,N,\\
U(\mathbf{v})^n = 0, \quad x \in \partial\Omega, \quad n = 0,1,\dots,N,\\
U(\mathbf{v})^0 = 0, \quad x \in \Omega,
\end{cases} \tag{4.1}$$

$$(4.2)\quad \begin{cases} {}^B\bar{D}_\tau^{1,x} Z(\mathbf{w})^{n-1} - \Delta {}^B\bar{D}_\tau^{1-\alpha,x} Z(\mathbf{w})^{n-1} = w^n - u_d^n, \quad x \in \Omega, \quad n = N, \dots, 1, \\ Z(\mathbf{w})^n = 0, \; x \in \partial\Omega, \quad n = N, \dots, 1, 0, \\ Z(\mathbf{w})^N = 0, \quad x \in \Omega, \end{cases}$$

where $f^n = \frac{1}{\tau}\int_{t_{n-1}}^{t_n} f(\cdot,t)\mathrm{d}t$, and $u_d^n = \frac{1}{\tau}\int_{t_{n-1}}^{t_n} u_d(\cdot,t)\mathrm{d}t$. Let $\mathbf{U}(\mathbf{v}) = (U(\mathbf{v})^n)_{n=1}^N$ and $\mathbf{Z}(\mathbf{w}) = (Z(\mathbf{w})^{n-1})_{n=1}^N$, the stability results for the system (4.1)-(4.2) are established in the following.

LEMMA 4.2. *Let $U(\mathbf{v})^n$ and $Z(\mathbf{w})^{n-1}$ be the solutions to the system (4.1)-(4.2), respectively. Then we have*

$$(4.3)\qquad |||\mathbf{U}(\mathbf{q}) - \mathbf{U}(\mathbf{v})||| \le C|||\mathbf{q} - \mathbf{v}|||,$$

$$(4.4)\qquad |||\mathbf{Z}(\mathbf{u}) - \mathbf{Z}(\mathbf{w})||| \le C|||\mathbf{u} - \mathbf{w}|||,$$

where $\mathbf{u} = (u(\cdot,t_n))_{n=1}^N$ and $\mathbf{q} = (q(\cdot,t_{n-1}))_{n=1}^N$.

Proof. By the estimate [11, Lemma 3.4] as follows:

$$(4.5)\qquad C_0|\xi|\tau \le |1 - e^{\xi\tau}| \le C_1|\xi|\tau \quad \forall\, \xi \in \Gamma_{\theta,\kappa}^\tau,$$

we derive from (3.18) and Lemma 4.1 that

$$\begin{aligned} \|F^\tau(t)\| &\le C\int_{\Gamma_{\theta,\kappa}^\tau} |e^{\xi t}| \cdot \left|\frac{\xi\tau}{e^{\xi\tau}-1}\right| \cdot \|(\delta_\tau(e^{-\tau\beta(\xi)})^\alpha - \Delta)^{-1}\| \cdot |\delta_\tau(e^{-\tau\beta(\xi)})^{\alpha-1}| \cdot |\mathrm{d}\xi| \\ &\le C\int_{\Gamma_{\theta,\kappa}^\tau} |e^{\xi t}| \cdot |\xi|^{-1}|\mathrm{d}\xi| \le C. \end{aligned} \qquad (4.6)$$

Let $q_\tau(\cdot,t)|_{[t_{n-1},t_n)} = q^{n-1}(\cdot)$ and $v_\tau(\cdot,t)|_{[t_{n-1},t_n)} = v^{n-1}(\cdot)$, it yields from (3.17) that

$$\begin{aligned} \|U^n(\mathbf{q}) - U^n(\mathbf{v})\|_{L^2(\Omega)} &\le C\int_0^{t_n} \|F^\tau(t_n - s)\| \cdot \|q_\tau(\cdot,s) - v_\tau(\cdot,s)\|_{L^2(\Omega)}\mathrm{d}s \\ &\le C\int_0^{t_n} \|q_\tau(\cdot,s) - v_\tau(\cdot,s)\|_{L^2(\Omega)}\mathrm{d}s, \end{aligned}$$

which directly derives that

$$\begin{aligned} |||\mathbf{U}(\mathbf{q}) - \mathbf{U}(\mathbf{v})|||^2 &\le C\tau\sum_{n=1}^N \Big(\int_0^{t_n} \|q_\tau(\cdot,s) - v_\tau(\cdot,s)\|_{L^2(\Omega)}\mathrm{d}s\Big)^2 \\ &\le C\tau\sum_{n=1}^N\sum_{j=1}^n \int_{t_{j-1}}^{t_j} \|q_\tau(\cdot,s) - v_\tau(\cdot,s)\|_{L^2(\Omega)}^2\mathrm{d}s \\ &= C\tau\sum_{n=1}^N\sum_{j=1}^n \int_{t_{j-1}}^{t_j} \|q^{j-1} - v^{j-1}\|_{L^2(\Omega)}^2\mathrm{d}s \\ &\le C|||\mathbf{q} - \mathbf{v}|||^2. \end{aligned}$$

By (3.20), (4.5) and Lemma 4.1, it leads to $\|E^\tau(t)\| \le C$. Then we can also obtain the estimate (4.4) from (3.19) by the similar technique for (4.3). ∎

4.2. Error estimates. In this subsection, we dedicate to establish the error estimates for the temporal semidiscrete scheme (3.1)-(3.2), as shown in Theorem 4.7.

LEMMA 4.3. *Let $F(\cdot)$, $F^\tau(\cdot)$, $E(\cdot)$ and $E^\tau(\cdot)$ be given by (2.16), (3.18), (2.19) and (3.20), respectively. Then we have*

$$\|F(t) - F^\tau(t)\| \le C\tau^{1-\epsilon} t^{-(1-\epsilon)} \quad \forall\ \epsilon \in [0,1],\ t \in (0,T], \tag{4.7}$$

$$\|E(t) - E^\tau(t)\| \le C\tau^{1-\epsilon} t^{-(1-\epsilon)} \quad \forall\ \epsilon \in [0,1],\ t \in (0,T]. \tag{4.8}$$

Proof. From (2.16) and (3.18), it easily yields that

$$F(t) - F^\tau(t) = \frac{1}{2\pi\mathbf{i}} \int_{\Gamma_{\theta,\kappa}\setminus\Gamma^\tau_{\theta,\kappa}} e^{\xi t}\hat{D}_1(\xi)\mathrm{d}\xi + \frac{1}{2\pi\mathbf{i}} \int_{\Gamma^\tau_{\theta,\kappa}} e^{\xi t}\hat{D}_2(\xi)\mathrm{d}\xi, \tag{4.9}$$

where

$$\begin{aligned}
&\hat{D}_1(\xi) = \big(\beta(\xi)^\alpha - \Delta\big)^{-1}\beta(\xi)^{\alpha-1},\\
&\hat{D}_2(\xi) = \big(\beta(\xi)^\alpha - \Delta\big)^{-1}\beta(\xi)^{\alpha-1} - \frac{\xi\tau}{e^{\xi\tau}-1}\big(\delta_\tau(e^{-\tau\beta(\xi)})^\alpha - \Delta\big)^{-1}\delta_\tau(e^{-\tau\beta(\xi)})^{\alpha-1}.
\end{aligned}$$

It has from [11, Lemma 3.4] that

$$\left|1 - \frac{\xi\tau}{e^{\xi\tau}-1}\right| = |\delta_\tau(e^{-\xi\tau})^{-1}(\delta_\tau(e^{-\xi\tau}) - \xi)| \le C|\xi|\tau \quad \forall\ \xi \in \Gamma^\tau_{\theta,\kappa}, \tag{4.10}$$

then we derive from (4.5), Lemmas 2.3 and 4.1 that

$$\|\hat{D}_1(\xi)\| \le C\|\big(\beta(\xi)^\alpha - \Delta\big)^{-1}\| \cdot |\beta(\xi)|^{\alpha-1} \le C|\beta(\xi)|^{-1} \le C|\xi|^{-1} \quad \forall\ \xi \in \Gamma_{\theta,\kappa}, \tag{4.11}$$

and

$$\begin{aligned}
\|\hat{D}_2(\xi)\| &\le \|\big(\beta(\xi)^\alpha - \Delta\big)^{-1}\beta(\xi)^{\alpha-1}\|\\
&\quad + \|\frac{\xi\tau}{e^{\xi\tau}-1}\big(\delta_\tau(e^{-\tau\beta(\xi)})^\alpha - \Delta\big)^{-1}\delta_\tau(e^{-\tau\beta(\xi)})^{\alpha-1}\|\\
&\le C(|\beta(\xi)|^{-1} + |\delta_\tau(e^{-\tau\beta(\xi)})|^{-1})\\
&\le C|\xi|^{-1} \quad \forall\ \xi \in \Gamma^\tau_{\theta,\kappa}.
\end{aligned} \tag{4.12}$$

Furthermore, by using Lemma 4.1 and the estimate (4.10), we have $\|\hat{D}_1(\xi)\| \le C\tau$ for any $\xi \in \Gamma_{\theta,\kappa}\setminus\Gamma^\tau_{\theta,\kappa}$, and

$$\begin{aligned}
\|\hat{D}_2(\xi)\| &= \|\big(\beta(\xi)^\alpha - \Delta\big)^{-1}\big(\beta(\xi)^{\alpha-1} - \delta_\tau(e^{-\tau\beta(\xi)})^{\alpha-1}\big)\|\\
&\quad + \|\big[\big(\beta(\xi)^\alpha - \Delta\big)^{-1} - \big(\delta_\tau(e^{-\tau\beta(\xi)})^\alpha - \Delta\big)^{-1}\big]\delta_\tau(e^{-\tau\beta(\xi)})^{\alpha-1}\|\\
&\quad + \left\|\Big(1 - \frac{\xi\tau}{e^{\xi\tau}-1}\Big)\big(\delta_\tau(e^{-\tau\beta(\xi)})^\alpha - \Delta\big)^{-1}\delta_\tau(e^{-\tau\beta(\xi)})^{\alpha-1}\right\|\\
&\le C\tau \quad \forall\ \xi \in \Gamma^\tau_{\theta,\kappa},
\end{aligned} \tag{4.13}$$

where it applies the following estimate

$$\begin{aligned}
&\|\big(\beta(\xi)^\alpha - \Delta\big)^{-1} - \big(\delta_\tau(e^{-\tau\beta(\xi)})^\alpha - \Delta\big)^{-1}\|\\
&= \|\big(\beta(\xi)^\alpha - \Delta\big)^{-1}\big(\beta(\xi)^\alpha - \delta_\tau(e^{-\tau\beta(\xi)})^\alpha\big)\big(\delta_\tau(e^{-\tau\beta(\xi)})^\alpha - \Delta\big)^{-1}\|
\end{aligned}$$

$$\leq C\tau|\xi|^{1-\alpha} \quad \forall\, \xi \in \Gamma^{\tau}_{\theta,\kappa}.$$

Hence, it infers from (4.11), (4.12) and (4.13) that

$$\|\hat{D}_1(\xi)\| \leq C\tau^{1-\epsilon}|\xi|^{-\epsilon} \quad \forall\, \xi \in \Gamma_{\theta,\kappa}\backslash\Gamma^{\tau}_{\theta,\kappa},\ \epsilon \in [0,1], \tag{4.14}$$

$$\|\hat{D}_2(\xi)\| \leq C\tau^{1-\epsilon}|\xi|^{-\epsilon} \quad \forall\, \xi \in \Gamma^{\tau}_{\theta,\kappa},\ \epsilon \in [0,1]. \tag{4.15}$$

Consequently, the result (4.7) is obtained from the above estimates and (4.9), and (4.8) can also be derived by the similar approach. ∎

LEMMA 4.4. *Let u be the solution to the state equation (2.1) and $U(\mathbf{q})^n$ be the solution to the discrete equation (4.1) for $v^{n-1} := q^{n-1} = q(\cdot, t_{n-1})$. Then we have*

$$|||\mathbf{u} - \mathbf{U}(\mathbf{q})||| \leq C l_\tau \tau,$$

where $\mathbf{U}(\mathbf{q}) = (U(\mathbf{q})^n)_{n=1}^N$ and $l_\tau = |\ln \tau|$.

Proof. From the solution representations in (2.15) and (3.17), it follows that

$$\begin{aligned} u(\cdot,t_n) - U(q)^n = &\int_0^{t_n} \big(F(t_n - s) - F^\tau(t_n - s)\big)\big(f(\cdot,s) + q(\cdot,s)\big)\mathrm{d}s \\ &+ \int_0^{t_n} F^\tau(t_n - s)\big(f(\cdot,s) - f_\tau(\cdot,s)\big)\mathrm{d}s \\ &+ \int_0^{t_n} F^\tau(t_n - s)\big(q(\cdot,s) - q_\tau(\cdot,s)\big)\mathrm{d}s \\ := &\, A^n + B^n + C^n, \end{aligned}$$

for $n = 1, 2, \ldots, N$, where $f_\tau(\cdot,t)|_{(t_{n-1},t_n]} = f^n$ as in (3.14) and $q_\tau(\cdot,t)|_{[t_{n-1},t_n)} = q^{n-1} = q(\cdot,t_{n-1})$. For the term A^n, we derive from (4.7), (2.25) and (4.6) that

$$\begin{aligned} \|A^n\|_{L^2(\Omega)} \leq &\, C\tau^{1-\epsilon}\int_0^{t_{n-1}} \frac{(t_n + \tau - s)^{1-\epsilon}}{(t_{n-1} + \tau - s)^{1-\epsilon}}(t_n + \tau - s)^{-(1-\epsilon)}\|f(\cdot,s) + q(\cdot,s)\|_{L^2(\Omega)}\mathrm{d}s \\ &+ C\tau^{1-\epsilon}\int_{t_{n-1}}^{t_n} (t_n + \tau - s)^{-(1-\epsilon)}\|f(\cdot,s) + q(\cdot,s)\|_{L^2(\Omega)}\mathrm{d}s \\ \leq &\, C\tau^{1-\epsilon}\int_0^T \mathbf{1}_{\{t_n > s\}}(t_n + \tau - s)^{-(1-\epsilon)}\|f(\cdot,s) + q(\cdot,s)\|_{L^2(\Omega)}\mathrm{d}s, \quad \epsilon \in (0,1), \end{aligned}$$

which implies that

$$\begin{aligned} &|||(A^n)_{n=1}^N||| = \Big(\tau\sum_{n=1}^N \|A^n\|^2_{L^2(\Omega)}\Big)^{\frac{1}{2}} \\ &\leq C\Big(\tau\sum_{n=1}^N \tau^{2-2\epsilon}\Big[\int_0^T \mathbf{1}_{\{t_n > s\}}(t_n + \tau - s)^{-(1-\epsilon)}\|f(\cdot,s) + q(\cdot,s)\|_{L^2(\Omega)}\mathrm{d}s\Big]^2\Big)^{\frac{1}{2}} \\ &\leq C\tau^{1-\epsilon}\Big(\tau\sum_{n=1}^N \int_0^T \mathbf{1}_{\{t_n > s\}}(t_n + \tau - s)^{-(1-\epsilon)}\mathrm{d}s \\ &\qquad\qquad \cdot \int_0^T \mathbf{1}_{\{t_n > s\}}(t_n + \tau - s)^{-(1-\epsilon)}\|f(\cdot,s) + q(\cdot,s)\|^2_{L^2(\Omega)}\mathrm{d}s\Big)^{\frac{1}{2}} \\ &\leq C\tau^{1-\epsilon}\Big(\epsilon^{-1}\tau\sum_{n=1}^N \int_0^T \mathbf{1}_{\{t_n > s\}}(t_n + \tau - s)^{-(1-\epsilon)}\|f(\cdot,s) + q(\cdot,s)\|^2_{L^2(\Omega)}\mathrm{d}s\Big)^{\frac{1}{2}} \end{aligned}$$

$$\leq C\tau^{1-\epsilon}\Big(\epsilon^{-2}\int_0^T \|f(\cdot,s)+q(\cdot,s)\|^2_{L^2(\Omega)}\mathrm{d}s\Big)^{\frac{1}{2}}$$
$$\leq C\tau^{1-\epsilon}\epsilon^{-1}\|f+q\|_{L^2(0,T;L^2(\Omega))}$$
$$\leq C\tau^{1-\epsilon}\epsilon^{-1} = Cl_\tau\tau,$$

where $\epsilon = l_\tau^{-1}$ is taken with $l_\tau = |\ln\tau|$, and it applies two inequalities [12] as follows:

$$\sup_{1\leq n\leq N}\int_0^T \mathbf{1}_{\{t_n>s\}}\,(t_n+\tau-s)^{-(1-\epsilon)}\,\mathrm{d}s \leq C\epsilon^{-1}\,(t_n+\tau)^{\epsilon} \leq C\epsilon^{-1}, \tag{4.16}$$

$$\sup_{s\in(0,T)}\tau\sum_{n=1}^N \mathbf{1}_{\{t_n>s\}}\,(t_n+\tau-s)^{-(1-\epsilon)} \leq \sup_{s\in(0,T)}\int_{s-\tau}^T (t+\tau-s)^{-(1-\epsilon)}\mathrm{d}t \leq C\epsilon^{-1}. \tag{4.17}$$

From (3.14) with $f^n = \frac{1}{\tau}\int_{t_{n-1}}^{t_n} f(\cdot,t)\mathrm{d}t$, we have that

$$\int_{t_{j-1}}^{t_j} F^\tau(t_n-t_{j-1})f_\tau(\cdot,s)\mathrm{d}s = \int_{t_{j-1}}^{t_j} F^\tau(t_n-t_{j-1})\frac{1}{\tau}\int_{t_{j-1}}^{t_j} f(\cdot,w)\mathrm{d}w\mathrm{d}s$$
$$= \int_{t_{j-1}}^{t_j} F^\tau(t_n-t_{j-1})f(\cdot,s)\mathrm{d}s,$$

and it also holds that

$$\|F^\tau(t_n-s)-F^\tau(t_n-t_{j-1})\|$$
$$\leq C\int_{\Gamma^\tau_{\theta,\kappa}} \big|e^{\xi(t_n-s)}-e^{\xi(t_n-t_{j-1})}\big|\cdot\Big|\frac{\xi\tau}{e^{\xi\tau}-1}\Big|$$
$$\cdot\,\big\|\big(\delta_\tau(e^{-\tau\beta(\xi)})^\alpha-\Delta\big)^{-1}\big\|\cdot|\delta_\tau(e^{-\tau\beta(\xi)})^{\alpha-1}|\cdot|\mathrm{d}\xi|$$
$$\leq C\int_{\Gamma^\tau_{\theta,\kappa}} |e^{\xi(t_n-s)}|\cdot|1-e^{\xi(s-t_{j-1})}|\cdot|\xi|^{-1}\cdot|\mathrm{d}\xi|$$
$$\leq C\int_{\Gamma^\tau_{\theta,\kappa}} |e^{\xi(t_n-s)}|\cdot\tau^{1-\epsilon}|\xi|^{-\epsilon}\cdot|\mathrm{d}\xi|$$
$$\leq C\tau^{1-\epsilon}(t_n-s)^{-(1-\epsilon)},\quad s\in(t_{j-1},t_j).$$

Then we derive from the above estimates and (4.6) that

$$\|B^n\|_{L^2(\Omega)} \leq \sum_{j=1}^n\int_{t_{j-1}}^{t_j}\|F^\tau(t_n-s)-F^\tau(t_n-t_{j-1})\|\cdot\|f(\cdot,s)-f_\tau(\cdot,s)\|_{L^2(\Omega)}\mathrm{d}s$$
$$\leq C\tau^{1-\epsilon}\int_0^{t_{n-1}}(t_n-s)^{-(1-\epsilon)}\|f(\cdot,s)-f_\tau(\cdot,s)\|_{L^2(\Omega)}\mathrm{d}s$$
$$+\int_{t_{n-1}}^{t_n}\|f(\cdot,s)-f_\tau(\cdot,s)\|_{L^2(\Omega)}\mathrm{d}s.$$

By the similar approach in the estimate of $|||(A^n)_{n=1}^N|||$, it obtains

$$|||(B^n)_{n=1}^N||| \leq C\tau^{1-\epsilon}\epsilon^{-1}\|f-f_\tau\|_{L^2(0,T;L^2(\Omega))} \leq C\tau^{1-\epsilon}\epsilon^{-1} \leq Cl_\tau\tau.$$

As for C^n, we have from (4.6) that

$$
\begin{aligned}
|||(C^n)_{n=1}^N||| &\le C\Big(\tau\sum_{n=1}^N\Big(\int_0^{t_n}\|q(\cdot,s)-q_\tau(\cdot,s)\|_{L^2(\Omega)}\mathrm{d}s\Big)^2\Big)^{\frac{1}{2}}\\
&= C\Big(\tau\sum_{n=1}^N\Big(\sum_{j=1}^n\int_{t_{j-1}}^{t_j}\|q(\cdot,s)-q(\cdot,t_{j-1})\|_{L^2(\Omega)}\mathrm{d}s\Big)^2\Big)^{\frac{1}{2}}\\
&\le C\Big(\tau\sum_{n=1}^N\tau^2\Big(\int_0^{t_n}\|\partial_s q(\cdot,s)\|_{L^2(\Omega)}\mathrm{d}s\Big)^2\Big)^{\frac{1}{2}}\\
&\le C\Big(\tau^2\int_0^T\|\partial_s q(\cdot,s)\|^2_{L^2(\Omega)}\mathrm{d}s\Big)^{\frac{1}{2}}\\
&\le C\tau\|q\|_{H^1(0,T;L^2(\Omega))}\le C\tau.
\end{aligned}
$$

Therefore, the result is derived by the above estimates. ∎

Let $Z(\mathbf{u})^{n-1}$ be the solution to the discrete equation (4.2) for $w^n := u^n = u(\cdot,t_n)$ and $u_d^n = \frac{1}{\tau}\int_{t_{n-1}}^{t_n}u_d(\cdot,t)\mathrm{d}t$. With (2.18) and (3.19), it follows that

$$
\begin{aligned}
z(\cdot,t_{n-1}) - Z(u)^{n-1} &= \int_{t_{n-1}}^T\big(E(s-t_{n-1})-E^\tau(s-t_{n-1})\big)\big(u(\cdot,s)-u_d(\cdot,s)\big)\mathrm{d}s\\
&\quad+\int_{t_{n-1}}^T E^\tau(s-t_{n-1})\big(u(\cdot,s)-u_\tau(\cdot,s)\big)\mathrm{d}s\\
&\quad-\int_{t_{n-1}}^T E^\tau(s-t_{n-1})\big(u_d(\cdot,s)-u_{d\tau}(\cdot,s)\big)\mathrm{d}s,
\end{aligned}
$$

where $u_\tau(\cdot,t)|_{(t_{n-1},t_n]} = u^n = u(\cdot,t_n)$ and $u_{d\tau}(\cdot,t)|_{(t_{n-1},t_n]} = u_d^n$ for $n=1,2,\ldots,N$. By the similar techniques to estimate A^n, B^n and C^n as above, we can also obtain the estimate as follows.

LEMMA 4.5. *Let z be the solution to the adjoint equation (2.2), and $\mathbf{Z}(\mathbf{u}) = (Z(\mathbf{u})^{n-1})_{n=1}^N$ with $Z(\mathbf{u})^{n-1}$ being the solution to the discrete equation (4.2) for $w^n := u^n = u(\cdot,t_n)$ and $u_d^n = \frac{1}{\tau}\int_{t_{n-1}}^{t_n}u_d(\cdot,t)\mathrm{d}t$. Then we have*

$$|||\mathbf{z}-\mathbf{Z}(\mathbf{u})||| \le Cl_\tau\tau,$$

where $\mathbf{z} = (z(\cdot,t_{n-1}))_{n=1}^N$ and $l_\tau = |\ln\tau|$.

By using the above results, the error analysis of $|||\mathbf{q}-\mathbf{Q}|||$ is derived in the following lemma.

LEMMA 4.6. *Let q and Q^{n-1} be solutions to (2.3) and (3.12), respectively. Then there exists a constant C proportional to $1/\gamma$ such that*

$$|||\mathbf{q}-\mathbf{Q}||| \le Cl_\tau\tau. \tag{4.18}$$

Proof. By (3.8) and (3.9), we have

$$
\begin{aligned}
[\mathbf{Z}-\mathbf{Z}(\mathbf{U}(\mathbf{q})),\mathbf{q}-\mathbf{Q}] &= [\mathbf{Z}-\mathbf{Z}(\mathbf{U}(\mathbf{q})),(\bar{D}_\tau^{1,x}-\Delta\bar{D}_\tau^{1-\alpha,x})(\mathbf{U}(\mathbf{q})-\mathbf{U})]\\
&= [({}^B\bar{D}_\tau^{1,x}-{}^B\bar{D}_\tau^{1-\alpha,x}\Delta)(\mathbf{Z}-\mathbf{Z}(\mathbf{U}(\mathbf{q}))),\mathbf{U}(\mathbf{q})-\mathbf{U}]\\
&= -|||\mathbf{U}(\mathbf{q})-\mathbf{U}|||^2 \le 0.
\end{aligned}
$$

It follows from (2.3) and (2.9) that

$$(4.19)\qquad \big(\gamma q(\cdot,t_{n-1})+z(\cdot,t_{n-1}),v-q(\cdot,t_{n-1})\big)\geq 0\quad \forall\ v\in L^2(\Omega),\ a\leq v\leq b.$$

Then we have from (4.19) and (3.12) that

$$\begin{aligned}&[\gamma\mathbf{q},\mathbf{q}-\mathbf{Q}]=-[\mathbf{z},\mathbf{q}-\mathbf{Q}]-[\gamma\mathbf{q}+\mathbf{z},\mathbf{Q}-\mathbf{q}]\leq-[\mathbf{z},\mathbf{q}-\mathbf{Q}],\\ &-[\gamma\mathbf{Q},\mathbf{q}-\mathbf{Q}]=[\mathbf{Z},\mathbf{q}-\mathbf{Q}]-[\gamma\mathbf{Q}+\mathbf{Z},\mathbf{q}-\mathbf{Q}]\leq[\mathbf{Z},\mathbf{q}-\mathbf{Q}],\end{aligned}$$

which further leads to

$$\begin{aligned}\gamma|||\mathbf{q}-\mathbf{Q}|||^2&=\gamma[\mathbf{q},\mathbf{q}-\mathbf{Q}]-\gamma[\mathbf{Q},\mathbf{q}-\mathbf{Q}]\\&\leq-[\mathbf{z},\mathbf{q}-\mathbf{Q}]+[\mathbf{Z},\mathbf{q}-\mathbf{Q}]\\&=[\mathbf{Z}-\mathbf{Z}(\mathbf{U}(\mathbf{q})),\mathbf{q}-\mathbf{Q}]+[\mathbf{Z}(\mathbf{U}(\mathbf{q}))-\mathbf{z},\mathbf{q}-\mathbf{Q}]\\&\leq[\mathbf{Z}(\mathbf{U}(\mathbf{q}))-\mathbf{z},\mathbf{q}-\mathbf{Q}].\end{aligned}$$

Therefore, it derives from the estimates in Lemmas 4.2, 4.4 and 4.5 that

$$\begin{aligned}|||\mathbf{q}-\mathbf{Q}|||&\leq C|||\mathbf{Z}(\mathbf{U}(\mathbf{q}))-\mathbf{z}|||\\&\leq C|||\mathbf{Z}(\mathbf{U}(\mathbf{q}))-\mathbf{Z}(\mathbf{u})|||+C|||\mathbf{Z}(\mathbf{u})-\mathbf{z}|||\\&\leq C|||\mathbf{U}(\mathbf{q})-\mathbf{u}|||+C|||\mathbf{Z}(\mathbf{u})-\mathbf{z}|||\\&\leq Cl_\tau\tau.\end{aligned}$$

∎

With the above discussions, we present the error estimate of the semidiscrete scheme (3.10)-(3.11), which is stated in the following theorem.

THEOREM 4.7. *Assume that* $f,u_d\in L^2(0,T;L^2(\Omega))$, $\mathrm{Re}(\rho U(x))\geq 0$ *and* $U(x)\in L^\infty(\Omega)$. *Let* (u,z,q) *and* (U^n,Z^{n-1},Q^{n-1}) *be the solutions of the problems* (2.1)-(2.3) *and* (3.10)-(3.12), *respectively, then we have*

$$|||\mathbf{u}-\mathbf{U}|||+|||\mathbf{z}-\mathbf{Z}|||+|||\mathbf{q}-\mathbf{Q}|||\leq Cl_\tau\tau,$$

where $\mathbf{u}=(u(\cdot,t_n))_{n=1}^N$, $\mathbf{z}=(z(\cdot,t_{n-1}))_{n=1}^N$, $\mathbf{q}=(q(\cdot,t_{n-1}))_{n=1}^N$, $l_\tau=|\ln\tau|$, *and the constant* C *depending on* $1/\gamma$ *is independent of* τ.

Proof. It follows from the estimates in Lemmas 4.2, 4.4 and 4.6 that

$$\begin{aligned}|||\mathbf{u}-\mathbf{U}|||&\leq|||\mathbf{u}-\mathbf{U}(\mathbf{q})|||+|||\mathbf{U}(\mathbf{q})-\mathbf{U}|||\\&\leq|||\mathbf{u}-\mathbf{U}(\mathbf{q})|||+C|||\mathbf{q}-\mathbf{Q}|||\\&\leq Cl_\tau\tau.\end{aligned}$$

By using the triangle inequality, Lemmas 4.2 and 4.5, we obtain

$$\begin{aligned}|||\mathbf{z}-\mathbf{Z}|||&\leq|||\mathbf{z}-\mathbf{Z}(\mathbf{u})|||+|||\mathbf{Z}(\mathbf{u})-\mathbf{Z}|||\\&\leq|||\mathbf{z}-\mathbf{Z}(\mathbf{u})|||+C|||\mathbf{u}-\mathbf{U}|||\\&\leq Cl_\tau\tau.\end{aligned}$$

Then the result is obtained together with Lemma 4.6. ∎

5. Numerical examples. In this section, we present two numerical examples to illustrate the efficiency of the semidiscrete scheme (3.10)-(3.11) for solving the optimal control problem (1.1)-(1.2) governed by the backward fractional Feynman-Kac equation, and verify the theoretical error estimate in Section 4.

EXAMPLE 1. *Let* $\Omega = (0,1)$*,* $T = 1$*,* $\gamma = 0.1$*,* $U(x) = x$*,* $\rho = 1$*,* $a = -5.0$ *and* $b = 0.0$*. The exact solutions* (u, z, q) *to the optimal control problem* (1.1)-(1.2) *in one dimension are chosen as*

$$u = e^{-t\rho x} t \sin(\pi x), \quad z = e^{t\rho x}(1-t)\sin(\pi x),$$
$$q = \max\{a, \min\{-z/\gamma, b\}\},$$

the functions f *and* u_d *are computed by* (2.1)*,* (2.2) *and the exact solutions.*

The discrete optimal control problem (3.1)-(3.2) is solved by the inexact alternating direction method of multipliers (ADMM) algorithm [8] with the piecewise linear finite element discretization in space, where the Lagrange penalty parameter is taken the same as the penalty parameter γ, and the stopping criterion is measured by the maximal of the primal and dual residuals as in [8, Section 6] with a prescribed tolerance being 1.0×10^{-5}. The mesh size $h = 1/64$ is chosen for the spatial finite element discretization. In Table 1, it reports the errors $|||\mathbf{u} - \mathbf{U}|||$, $|||\mathbf{z} - \mathbf{Z}|||$, $|||\mathbf{q} - \mathbf{Q}|||$ and the temporal convergence orders for Example 1 with $\alpha = 0.2, 0.5, 0.8$ and $\tau = 1/4, 1/8, 1/16, 1/32, 1/64$. First order convergence in time is observed for different values of α, which confirms the theoretical result in Theorem 4.7 and the efficiency of our numerical scheme.

TABLE 1
The errors $|||\mathbf{u} - \mathbf{U}|||$*,* $|||\mathbf{z} - \mathbf{Z}|||$*,* $|||\mathbf{q} - \mathbf{Q}|||$ *and the convergence orders for Example 1.*

α	Error	τ =1/4	τ =1/8	τ =1/16	τ =1/32	τ =1/64	Order
0.2	$\|\|\|\mathbf{u} - \mathbf{U}\|\|\|$	2.27e-02	1.11e-02	5.18e-03	2.47e-03	1.18e-03	≈ 1.07 (1.0)
	$\|\|\|\mathbf{z} - \mathbf{Z}\|\|\|$	2.19e-02	1.13e-02	5.62e-03	2.76e-03	1.35e-03	≈ 1.01 (1.0)
	$\|\|\|\mathbf{q} - \mathbf{Q}\|\|\|$	1.70e-01	9.09e-02	4.56e-02	2.22e-02	1.07e-02	≈ 1.00 (1.0)
0.5	$\|\|\|\mathbf{u} - \mathbf{U}\|\|\|$	3.42e-02	1.71e-02	8.34e-03	4.08e-03	2.00e-03	≈ 1.02 (1.0)
	$\|\|\|\mathbf{z} - \mathbf{Z}\|\|\|$	3.15e-02	1.62e-02	8.11e-03	4.04e-03	2.02e-03	≈ 0.99 (1.0)
	$\|\|\|\mathbf{q} - \mathbf{Q}\|\|\|$	2.72e-01	1.45e-01	7.36e-02	3.70e-02	1.85e-02	≈ 0.97 (1.0)
0.8	$\|\|\|\mathbf{u} - \mathbf{U}\|\|\|$	4.77e-02	2.37e-02	1.18e-02	5.81e-03	2.87e-03	≈ 1.01 (1.0)
	$\|\|\|\mathbf{z} - \mathbf{Z}\|\|\|$	5.49e-02	2.81e-02	1.43e-02	7.22e-03	3.65e-03	≈ 0.98 (1.0)
	$\|\|\|\mathbf{q} - \mathbf{Q}\|\|\|$	4.17e-01	2.27e-01	1.16e-01	5.94e-02	3.01e-02	≈ 0.95 (1.0)

EXAMPLE 2. *Let* $\Omega = (0,1)^2$*,* $T = 1$*,* $\gamma = 1$*,* $U(x,y) = x + y$*,* $\rho = 1$*,* $a = -0.2$ *and* $b = 0.0$*. We choose the exact solutions* (u, z, q) *to the optimal control problem* (1.1)-(1.2) *in two dimensions as*

$$u = e^{-t\rho(x+y)} t \sin(\pi x)\sin(\pi y),$$
$$z = e^{t\rho(x+y)-1}(1-t)\sin(\pi x)\sin(\pi y),$$
$$q = \max\{a, \min\{-z/\gamma, b\}\},$$

and calculate f *and* u_d *by* (2.1)*,* (2.2) *and the exact solutions.*

We fix the uniform triangular mesh with the mesh size $h = 1/32$ over the domain $\Omega = (0,1)^2$ in Example 2, and solve the discrete problem (3.1)-(3.2) by the inexact

ADMM algorithm [8] with the same settings as in Example 1. For $\alpha = 0.2, 0.5, 0.8$ and $\tau = 1/4, 1/8, 1/16, 1/32, 1/64$, the errors $|||\mathbf{u} - \mathbf{U}|||$, $|||\mathbf{z} - \mathbf{Z}|||$, $|||\mathbf{q} - \mathbf{Q}|||$ and the temporal convergence orders are presented in Table 2, from which a first order convergence order is observed in the time direction. This is also consistent with the theoretical analysis in Theorem 4.7, and illustrates the effectiveness of the proposed scheme as well.

TABLE 2
The errors $|||\mathbf{u} - \mathbf{U}|||$, $|||\mathbf{z} - \mathbf{Z}|||$, $|||\mathbf{q} - \mathbf{Q}|||$ and the convergence orders for Example 2.

α	Error	τ =1/4	τ =1/8	τ =1/16	τ =1/32	τ =1/64	Order
0.2	$\|\|\|\mathbf{u} - \mathbf{U}\|\|\|$	9.86e-03	5.06e-03	2.53e-03	1.23e-03	5.83e-04	$\approx$ 1.02 (1.0)
	$\|\|\|\mathbf{z} - \mathbf{Z}\|\|\|$	5.14e-02	2.50e-02	1.20e-02	5.76e-03	2.80e-03	$\approx$ 1.05 (1.0)
	$\|\|\|\mathbf{q} - \mathbf{Q}\|\|\|$	4.85e-02	2.38e-02	1.14e-02	5.50e-03	2.67e-03	$\approx$ 1.05 (1.0)
0.5	$\|\|\|\mathbf{u} - \mathbf{U}\|\|\|$	1.08e-02	5.71e-03	2.88e-03	1.43e-03	7.11e-04	$\approx$ 0.98 (1.0)
	$\|\|\|\mathbf{z} - \mathbf{Z}\|\|\|$	4.90e-02	2.34e-02	1.11e-02	5.33e-03	2.62e-03	$\approx$ 1.06 (1.0)
	$\|\|\|\mathbf{q} - \mathbf{Q}\|\|\|$	4.64e-02	2.22e-02	1.05e-02	5.05e-03	2.47e-03	$\approx$ 1.06 (1.0)
0.8	$\|\|\|\mathbf{u} - \mathbf{U}\|\|\|$	1.70e-02	9.03e-03	4.64e-03	2.36e-03	1.20e-03	$\approx$ 0.96 (1.0)
	$\|\|\|\mathbf{z} - \mathbf{Z}\|\|\|$	4.85e-02	2.37e-02	1.16e-02	5.79e-03	2.95e-03	$\approx$ 1.01 (1.0)
	$\|\|\|\mathbf{q} - \mathbf{Q}\|\|\|$	4.47e-02	2.19e-02	1.07e-02	5.32e-03	2.69e-03	$\approx$ 1.01 (1.0)

6. Conclusion. This work investigates the theoretical and numerical issues for an optimal control problem governed by the backward fractional Feynman-Kac equation, which governs the probability density function of functionals in anomalous and multiscale diffusion. Due to time-space coupled nonlocal fractional substantial derivative in the equation and its noncommutativity with the Laplacian, it confronts significant difficulties. The well-posedness, optimality conditions and solution regularity of the optimal control problem are established. Subsequently, a temporal semidiscrete scheme is proposed for the optimal control problem, where the Riemann-Liouville fractional substantial derivative in time is discretized by the BECQ formula. We rigorously conduct the temporal error estimate based on the regularity results of the solution, demonstrating a first-order convergence order, which is supported by the numerical results. It is noticed that the spatial error analysis of the finite element method for the optimal control problem still encounters numerous challenges, which remains to be addressed in future work.

REFERENCES

[1] H. Antil, T. Brown, R. Khatri, A. Onwunta, D. Verma, and M. Warma. Optimal control, numerics, and applications of fractional PDEs. In *Numerical control. Part A*, volume 23 of *Handbook of Numerical Analysis*, pages 87–114. North-Holland, Amsterdam, 2022.

[2] S. Carmi, L. Turgeman, and E. Barkai. On distributions of functionals of anomalous diffusion paths. *J. Stat. Phys.*, 141(6):1071–1092, 2010.

[3] M. Chen and W. H. Deng. Discretized fractional substantial calculus. *ESAIM Math. Model. Numer. Anal.*, 49(2):373–394, 2015.

[4] W. Deng, R. Hou, W. Wang, and P. Xu. *Modeling Anomalous Diffusion: From Statistics to Mathematics.* World Scientific, 2020.

[5] W. H. Deng, M. H. Chen, and E. Barkai. Numerical algorithms for the forward and backward fractional Feynman-Kac equations. *J. Sci. Comput.*, 62(3):718–746, 2015.

[6] W. H. Deng, B. Li, Z. Qian, and H. Wang. Time discretization of a tempered fractional Feynman-Kac equation with measure data. *SIAM J. Numer. Anal.*, 56(6):3249–3275, 2018.

[7] R. Friedrich, F. Jenko, A. Baule, and S. Eule. Anomalous diffusion of inertial, weakly damped particles. *Phys. Rev. Lett.*, 96(23):230601, 2006.

[8] R. Glowinski, Y. Song, X. Yuan, and H. Yue. Application of the alternating direction method of multipliers to control constrained parabolic optimal control problems and beyond. *Ann. Appl. Math.*, 38(2):115–158, 2022.
[9] I. Golding and E. C. Cox. Physical nature of bacterial cytoplasm. *Phys. Rev. Lett.*, 96(9):098102, 2006.
[10] M. Gunzburger, B. Li, and J. Wang. Convergence of finite element solutions of stochastic partial integro-differential equations driven by white noise. *Numer. Math.*, 141(4):1043–1077, 2019.
[11] M. Gunzburger, B. Li, and J. Wang. Sharp convergence rates of time discretization for stochastic time-fractional PDEs subject to additive space-time white noise. *Math. Comp.*, 88(318):1715–1741, 2019.
[12] M. Gunzburger and J. Wang. Error analysis of fully discrete finite element approximations to an optimal control problem governed by a time-fractional PDE. *SIAM J. Control Optim.*, 57(1):241–263, 2019.
[13] L. Hao and W. Y. Tian. Analysis of a WSGD scheme for backward fractional Feynman-Kac equation with nonsmooth data. *Adv. Comput. Math.*, 50(4):Paper No. 87, 26, 2024.
[14] L. Hao and W. Y. Tian. Numerical discretization and error analysis for an optimal control problem governed by forward fractional Feynman-Kac equation. *J. Sci. Comput.*, 105(3):Paper No. 71, 26, 2025.
[15] B. Jin, B. Li, and Z. Zhou. Pointwise-in-time error estimates for an optimal control problem with subdiffusion constraint. *IMA J. Numer. Anal.*, 40(1):377–404, 2020.
[16] M. Kac. On distributions of certain Wiener functionals. *Trans. Amer. Math. Soc.*, 65:1–13, 1949.
[17] D. Kinderlehrer and G. Stampacchia. *An introduction to variational inequalities and their applications*, volume 31 of *Classics in Applied Mathematics*. SIAM, Philadelphia, PA, 2000. Reprint of the 1980 original.
[18] C. Li, W. Deng, and L. Zhao. Well-posedness and numerical algorithm for the tempered fractional differential equations. *Discrete Contin. Dyn. Syst. Ser. B*, 24(4):1989–2015, 2019.
[19] X. J. Li and C. J. Xu. Existence and uniqueness of the weak solution of the space-time fractional diffusion equation and a spectral method approximation. *Commun. Comput. Phys.*, 8(5):1016–1051, 2010.
[20] Y. Li, H. Wang, and X. Zheng. Analysis and simulation of optimal control for a two-time-scale fractional advection-diffusion-reaction equation with space-time-dependent order and coefficients. *Multiscale Model. Simul.*, 21(4):1690–1716, 2023.
[21] C. Lubich. Discretized fractional calculus. *SIAM J. Math. Anal.*, 17(3):704–719, 1986.
[22] R. Metzler and J. Klafter. The random walk's guide to anomalous diffusion: a fractional dynamics approach. *Phys. Rep.*, 339(1):1–77, 2000.
[23] R. Metzler and J. Klafter. The restaurant at the end of the random walk: recent developments in the description of anomalous transport by fractional dynamics. *J. Phys. A*, 37(31):R161–R208, 2004.
[24] G. M. Mophou and G. M. N'Guérékata. Optimal control of a fractional diffusion equation with state constraints. *Comput. Math. Appl.*, 62(3):1413–1426, 2011.
[25] D. Nie, J. Sun, and W. Deng. Numerical methods for forward fractional Feynman-Kac equation. *Adv. Comput. Math.*, 50(3):Paper No. 58, 40, 2024.
[26] I. Podlubny. *Fractional Differential Equations*. Academic Press, San Diego, 1999.
[27] D. A. Raichlen, B. M. Wood, A. D. Gordon, A. Z. P. Mabulla, F. W. Marlowe, and H. Pontzer. Evidence of Lévy walk foraging patterns in human hunter-gatherers. *Proc. Natl. Acad. Sci. USA*, 111(2):728–733, 2014.
[28] Y. Sagi, M. Brook, I. Almog, and N. Davidson. Observation of anomalous diffusion and fractional self-similarity in one dimension. *Phys. Rev. Lett.*, 108(9):093002, 2012.
[29] J. M. Sancho, A. M. Lacasta, K. Lindenberg, I. M. Sokolov, and A. H. Romero. Diffusion on a solid surface: Anomalous is normal. *Phys. Rev. Lett.*, 92(25):250601, 2004.
[30] J. Sun, D. Nie, and W. Deng. Error estimates for backward fractional Feynman-Kac equation with non-smooth initial data. *J. Sci. Comput.*, 84(1):Paper No. 6, 23, 2020.
[31] J. Sun, D. Nie, and W. Deng. High-order BDF fully discrete scheme for backward fractional Feynman-Kac equation with nonsmooth data. *Appl. Numer. Math.*, 161:82–100, 2021.
[32] V. Thomée. *Galerkin Finite Element Methods for Parabolic Problems*. Springer-Verlag, Berlin, second edition, 2006.
[33] W. Y. Tian, H. Zhou, and W. H. Deng. A class of second order difference approximation for solving space fractional diffusion equations. *Math. Comp.*, 84(294):1703–1727, 2015.
[34] L. Turgeman, S. Carmi, and E. Barkai. Fractional Feynman-Kac equation for non-Brownian functionals. *Phys. Rev. Lett.*, 103(19):190201, 2009.

[35] T. Wang, B. Li, and X. Xie. Discontinuous Galerkin method for a distributed optimal control problem governed by a time fractional diffusion equation. *Comput. Math. Appl.*, 128:1–11, 2022.
[36] W. Wyss. The fractional diffusion equation. *J. Math. Phys.*, 27(11):2782–2785, 1986.
[37] X. Ye and C. Xu. Spectral optimization methods for the time fractional diffusion inverse problem. *Numer. Math. Theory Methods Appl.*, 6(3):499–516, 2013.
[38] Z. Zhou and W. Gong. Finite element approximation of optimal control problems governed by time fractional diffusion equation. *Comput. Math. Appl.*, 71(1):301–318, 2016.