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TIME DISCRETIZATION OF A TEMPERED FRACTIONAL FEYNMAN–KAC EQUATION WITH MEASURE DATA*

WEIHUA DENG†, BUYANG LI‡, ZHI QIAN§, AND HONG WANG¶

Abstract. A feasible approach to study tempered anomalous dynamics is to analyze its functional distribution, which is governed by the tempered fractional Feynman–Kac equation. The main challenges of numerically solving the equation come from the time-space coupled nonlocal operators and the complex parameters involved. In this work, we introduce an efficient time-stepping method to discretize the tempered fractional Feynman–Kac equation by using the Laplace transform representation of convolution quadrature. Rigorous error estimate for the discrete solutions is carried out in the measure norm. Numerical experiments are provided to support the theoretical results.

Key words. tempered fractional operators, Feynmann–Kac equation, integral representation, convolution quadrature, convergence

AMS subject classifications. 65M12, 65R20, 65Z05

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1. Introduction.

The phenomenon of diffusion occurs ubiquitously in nature. While Fick first set up the diffusion equation, it was Einstein who derived the diffusion equation from first principles [7]. Pearson modeled the diffusion process via random walk under the same assumptions as Einstein: (i) the existence of a mean free path and (ii) the existence of a mean waiting time of particles between collisions [31]. In this case, a particle's motion of independent jumps has no spatial correlation, and the variance of a particle excursion distance is finite. Consequently, the central limit theorem implies that the probability density function $p(x,t)$ of finding a particle at position x satisfies a normal distribution at any time t, and so, a diffusion equation.

In the last few decades more and more diffusion processes were found to be non-Fickian. For example, for a diffusive process in a heterogeneous medium, the particles may be absorbed to a low permeability zone which has a longer waiting time and leads to a subdiffusive process. The macroscopic dynamic equations for describing the distribution of the particles undergoing an anomalous subdiffusive process have been derived in [27]. For instance, the following time-fractional diffusion equation

$$\partial_t u - \Delta \partial_t^{1-\alpha} u = 0, \quad \alpha \in (0,1), \tag{1.1}$$

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†School of Mathematics and Statistics, Gansu Key Laboratory of Applied Mathematics and Complex Systems, Lanzhou University, Lanzhou 730000, People's Republic of China (dengwh@lzu.edu.cn).
‡Department of Applied Mathematics, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong (buyang.li@polyu.edu.hk).
§Department of Mathematics, Nanjing University, Nanjing 210093, People's Republic of China (zqian@nju.edu.cn).
¶Department of Mathematics, University of South Carolina, Columbia, SC 29208 (hwang@math.sc.edu).

and its alternative formulation

$$\partial_t^\alpha u - \Delta u = 0, \qquad \alpha \in (0,1), \tag{1.2}$$

have been used to model subdiffusive processes [3, 14, 25, 27], where $\partial_t^{1-\alpha} u$ in (1.1) denotes the Riemann–Liouville fractional derivative of order α, defined by

$$\partial_t^{1-\alpha} u(t) := \frac{1}{\Gamma(\alpha)} \frac{\mathrm{d}}{\mathrm{d}t} \int_0^t (t-s)^{\alpha-1} u(s)\,\mathrm{d}s \tag{1.3}$$

with $\Gamma(\xi) := \int_0^\infty s^{\xi-1} e^{-s} \mathrm{d}s$ denoting the Gamma function, and $\partial_t^\alpha u$ in (1.2) denotes the Caputo fractional derivative of order α, defined by

$$\partial_t^\alpha u(t) := \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} \partial_s u(s)\,\mathrm{d}s. \tag{1.4}$$

The Riemann–Liouville and Caputo fractional derivatives agree when $u(0) = 0$.

The functionals of the trajectories of tempered anomalous diffusions, a special kind of statistical quantity, appear in a wide range of problems across different fields ranging from probability theory, finance, data analysis, disordered systems, and computer science. Since the statistical quantities are random variables, it is interesting to know their probability distribution functions. The probability distribution functions can be obtained by solving the tempered fractional Feymann–Kac equation

$$D_t(x)G(x,t) - (\lambda^\alpha + \Delta) D_t(x)^{1-\alpha} G(x,t) = -G_0(x)(\lambda^\alpha D_t(x)^{1-\alpha} - \lambda) e^{ipU(x)t}, \tag{1.5}$$

which was derived in [38] (we refer to [37] for the case $\lambda = 0$), where $D_t(x) := \lambda - ipU(x) + \frac{\partial}{\partial t}$ is the substantial derivative, and $G_0(x)$ is a prescribed initial datum. The solution $G(x,t) = G(x,t;p)$, depending on the parameter p, represents the characteristic function of the joint probability density function $\rho(x,t;A)$ of finding a particle at position x and time t with functional value $\int_0^t U(x(\tau))d\tau = A$, i.e., $G(x,t;p) = \int_{\mathbb{R}} e^{-ipA} \rho(x,t;A)\mathrm{d}A$. The Riemann–Liouville fractional substantial derivative $D_t(x)^{1-\alpha}$ with $\alpha \in (0,1)$, is defined by

$$\begin{aligned} D_t(x)^{1-\alpha} G(x,t) &= \left(\lambda - ipU(x) + \frac{\partial}{\partial t}\right)^{1-\alpha} G(x,t) \\ &= \frac{1}{\Gamma(\alpha)} \left(\lambda - ipU(x) + \frac{\partial}{\partial t}\right) \int_0^t \frac{e^{-(t-s)(\lambda - ipU(x))}}{(t-s)^{1-\alpha}} G(x,s)\mathrm{d}s. \end{aligned} \tag{1.6}$$

The tempering exponent λ controls the rate of the transition from an anomalous diffusion to a normal diffusion. The function $U(x)$ is usually determined by a specific application [37].

Due to their wide applications, fractional evolution partial differential equations (FPDEs) have generated much interest in developing stable and accurate numerical methods as well as rigorous mathematical and numerical analysis. Various efficient time discretization methods have been proposed for solving these problems, including finite difference methods [6, 8, 12, 17, 29], convolution quadrature [5, 13, 21, 33], and discontinuous Galerkin stepping schemes [23, 24, 28]. The main difficulty of solving such problems is to achieve the desired accuracy for solutions which are weakly singular at $t = 0$. To overcome this difficluty, the error estimates in [5, 13, 21, 24, 29, 33] were carried out based only on the regularity of the initial data and source term without extra assumptions on the regularity of the solutions. These articles mainly focus on the models (1.1) and (1.2); see [16] on a fractional Fokker–Planck equation.

The tempered fractional Feynman–Kac equation (1.5) presents new mathematical difficulties that were not encountered in the FPDEs mentioned above. In particular, both the complex-valued function $ipU(x)$ involved in the fractional substantial derivative and the noncommutativity of the time and space partial differential operators, i.e., $\Delta D_t(x)^{1-\alpha} \neq D_t(x)^{1-\alpha}\Delta$, lead to difficulties in the analysis of the resolvent operator (on the Laplace transform side)

$$\big((\lambda - ipU(x) + z) - (\lambda^\alpha + \Delta)(\lambda - ipU(x) + z)^{1-\alpha}\big)^{-1}, \tag{1.7}$$

whose boundedness is crucial for the analysis of time discretization of (1.5). As a result, the existing numerical analysis of (1.1) and (1.2), as well as the analysis of the fractional Fokker–Planck equation [16], cannot be directly carried over to (1.5). To our best knowledge, no rigorous numerical analysis of the tempered fractional Feynman–Kac equation (1.5) is available in the literature despite its wide potential applications in describing the slow transition from anomalous diffusion to normal diffusion [4, 26, 36], solving occupation time in the half-space [22], first passage time [32], maximal displacement [35], and fluctuations of the occupation fraction [9] for the space and time-tempered anomalous diffusion.

The objective of this paper is to introduce an efficient time discretization method for solving (1.5), with rigorous analysis of the stability and convergence of the numerical solutions. We consider (1.5) in a bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$, $d \geq 1$, with the initial condition

$$G(x, 0) = G_0(x),\ x \in \Omega, \tag{1.8}$$

and the Dirichlet boundary condition

$$G(x, t) = 0,\ (x, t) \in \partial\Omega \times (0, T], \tag{1.9}$$

which means that the particles are absorbed when they reach the boundary. Consistent with the physical meaning of the solution, we assume that the initial datum G_0 is an arbitrary finite signed measure on Ω. Thus G_0 may not be a pointwise defined function. For example, G_0 can be a δ-function placed at the origin, which models the situation that the particles are initially concentrated at the origin. Recall that the space of finite signed measures on Ω, denoted by $M(\Omega)$, is the dual space of $C(\overline{\Omega})$ (the space of continuous functions on $\overline{\Omega}$); see [15, Appendix A]. We assume that α, λ, and p are fixed constants and U a given function defined on Ω with

$$\alpha \in (0, 1), \quad \lambda \geq 0, \quad p \in \mathbb{R}, \quad U \in C(\overline{\Omega}), \quad \text{and} \quad G_0 \in M(\Omega). \tag{1.10}$$

Under these assumptions, we prove the following error estimate for the numerical solution $G_N(x)$ at $t_N = T$:

$$\|G(\cdot, T) - G_N\|_{M(\Omega)} \leq c_T \|G_0\|_{M(\Omega)}\tau, \tag{1.11}$$

where $\tau = T/N$ denotes the step size of time discretization, and $\|\cdot\|_{M(\Omega)}$ simply denotes the dual norm of $C(\overline{\Omega})$, i.e.,

$$\|\phi\|_{M(\Omega)} := \sup_{\substack{f \in C(\overline{\Omega}) \\ \|f\|_{C(\overline{\Omega})} \leq 1}} |(f, \phi)|. \tag{1.12}$$

The error estimate above depends only on the measure of the initial data, without extra regularity assumption on the solution of the PDE. The derivation and analysis of the numerical scheme are based on Lubich's Laplace transform representation of convolution quadrature [18, 20], where the main difficulty is the analysis of the resolvent operator (1.7) and its discrete approximation.

The rest of this paper is organized as follows. In section 2, we illustrate our methodology on the basic fractional diffusion equation (1.1). In section 3, we extend the analysis in section 2 to the tempered fractional Feynman–Kac equation (1.5), and point out the key differences. The technical proofs for the analyticity and boundedness of the continuous and discrete resolvent operators of the tempered fractional Feynman–Kac equation are presented in section 4. In the last section, we present numerical examples to support the theoretical results proved in this paper.

2. Illustration of our methodology on the model (1.1). For the readers' convenience, we first illustrate our method of analysis on the basic fractional diffusion equation (1.1) under the boundary and initial conditions

$$\begin{aligned} u &= 0 \quad \text{on } \partial\Omega \times \mathbb{R}_+, \\ u(\cdot,0) &= u_0 \quad \text{in } \Omega, \end{aligned} \tag{2.1}$$

by using the Laplace transform and convolution quadrature techniques for the numerical analysis of (1.1); see [5, 21]. We then extend the analysis to the tempered fractional Feynman–Kac equation (1.5) in the next section by pointing out the key differences.

2.1. Derivation of the time-stepping scheme. The idea is to consider the Laplace transform (in time) of (1.1), namely,

$$(z - z^{1-\alpha}\Delta)\widehat{u}(x,z) = u_0(x), \tag{2.2}$$

where $\widehat{u}(x,z) = \int_0^\infty e^{-tz}u(x,t)\mathrm{d}t$ denotes the Laplace transform of $u(x,t)$ with respect to t. The last equation can be rewritten as

$$z^{1-\alpha}(z^\alpha - \Delta)\widehat{u}(x,z) = u_0(x). \tag{2.3}$$

Let $t_n = n\tau$, $n = 0,1,\dots,N$, be a uniform partition of the time interval $[0,T]$, with step size $\tau = T/N$, and let $u_n(x)$ denote the approximation of $u(x,t_n)$. By denoting $\zeta = e^{-\tau z}$, we approximate z, $\widehat{u}(\cdot,z)$, and u_0 in (2.3) by $\frac{1-\zeta}{\tau}$, $\tau\sum_{n=1}^\infty u_n\zeta^n$, and ζu_0, respectively. This gives us the following equation:

$$\left(\frac{1-\zeta}{\tau}\right)^{1-\alpha}\left(\left(\frac{1-\zeta}{\tau}\right)^{\alpha} - \Delta\right)\sum_{n=1}^\infty u_n\zeta^n = \frac{\zeta}{\tau}u_0. \tag{2.4}$$

If we let $b_j^{(\alpha)}$, $j = 0,1,2,\dots$, denote the coefficients in the power series expansion

$$(1-\zeta)^\alpha = \sum_{j=0}^\infty b_j^{(\alpha)}\zeta^j \tag{2.5}$$

and approximate the Riemann–Liouville fractional derivative ∂_t^α by (the backward Euler convolution quadrature)

$$\overline{\partial_\tau}^\alpha u_n = \frac{1}{\tau^\alpha}\sum_{j=1}^n b_{n-j}^{(\alpha)}u_j, \tag{2.6}$$

then straightforward calculation of the coefficients of the following product series yields

$$\left(\frac{1-\zeta}{\tau}\right)^{\alpha}\sum_{n=1}^{\infty}u_n\zeta^n=\frac{1}{\tau^{\alpha}}\left(\sum_{j=0}^{\infty}b_j^{(\alpha)}\zeta^j\right)\sum_{n=1}^{\infty}u_n\zeta^n=\sum_{n=1}^{\infty}(\overline{\partial_\tau}^{\alpha}u_n)\zeta^n. \tag{2.7}$$

Consequently, by expanding (2.4) into a power series of ζ and considering the coefficients of the power series on both sides, we obtain the following time-stepping scheme:

$$\overline{\partial_\tau}^{1-\alpha}(\overline{\partial_\tau}^{\alpha}-\Delta)u_n=\begin{cases}\tau^{-1}u_0 & \text{if } n=1,\\ 0 & \text{if } n\geq 2.\end{cases} \tag{2.8}$$

By using the product rule

$$\overline{\partial_\tau}^{1-\alpha}\overline{\partial_\tau}^{\alpha}u_n=\begin{cases}\tau^{-1}u_1 & \text{if } n=1,\\ \tau^{-1}(u_n-u_{n-1}) & \text{if } n\geq 2,\end{cases} \tag{2.9}$$

the last equation reduces to

$$\begin{aligned}\tau^{-1}u_1-\overline{\partial_\tau}^{1-\alpha}\Delta u_1&=\tau^{-1}u_0 \quad \text{if } n=1,\\ \frac{u_n-u_{n-1}}{\tau}-\overline{\partial_\tau}^{1-\alpha}\Delta u_n&=0 \qquad\quad \text{if } n\geq 2,\end{aligned} \tag{2.10}$$

which coincidently agrees with the following backward Euler convolution quadrature method considered in [21]:

$$\frac{u_n-u_{n-1}}{\tau}-\overline{\partial_\tau}^{1-\alpha}\Delta u_n=0. \tag{2.11}$$

This coincidence is due to our special construction of (2.4) in approximating (2.3). In section 3, we apply the methodology described above to derive an efficient time-stepping scheme for the tempered fractional Feynman–Kac equation (1.5). In contrast with (1.1), due to the complex structure of this physical model, the time-stepping scheme derived for (1.5) is no longer equivalent to the standard backward Euler convolution quadrature discretization of (1.5).

Remark 2.1. The scheme (2.11) can be used for practical computation, while (2.4) can be used for estimating the error of the numerical solutions. Since the inverse Laplace transforms of $z^{1-\alpha}\widehat{u}$ and $z^{\alpha}\widehat{u}$ do not involve any initial data of u, we choose to approximate (2.3) rather than approximating (2.2) directly. Starting with approximating (2.3) makes it easier to preserve the structure of the PDE on the Laplace transform side, thus more convenient for estimating the error of the numerical solutions (especially for the complex model (1.5) to be considered in this paper).

2.2. Error estimate. In this subsection, we illustrate the idea of the error estimate in [21]. We present a complete proof for comparison with the analysis of (1.5) in the next section. To this end, we note that for $\theta\in(\frac{\pi}{2},\pi)$ sufficiently close to $\frac{\pi}{2}$ the following estimates hold:

(2.12)

$$c_1|z|\leq\left|\frac{1-e^{-\tau z}}{\tau}\right|\leq c_2|z| \qquad \forall\, z\in\Sigma_\theta,\ |\mathrm{Im}(z)|\leq\frac{\pi}{\tau} \quad \text{(by Taylor expansion)},$$

$$\left|\frac{1-e^{-\tau z}}{\tau}-z\right|\leq c\tau|z|^2 \qquad \forall\, z\in\Sigma_\theta,\ |\mathrm{Im}(z)|\leq\frac{\pi}{\tau}\ \ \text{(by Taylor expansion)}, \tag{2.13}$$

$$\left|\left(\frac{1-e^{-\tau z}}{\tau}\right)^\alpha-z^\alpha\right|\leq c\tau|z|^{1+\alpha} \quad \forall\, z\in\Sigma_\theta,\ |\mathrm{Im}(z)|\leq\frac{\pi}{\tau}\ \ \text{(by Taylor expansion)}, \tag{2.14}$$

$$\left(\frac{1-e^{-\tau z}}{\tau}\right)^\alpha\in\Sigma_\theta \qquad \forall\, z\in\Sigma_\theta,\ |\mathrm{Im}(z)|\leq\frac{\pi}{\tau}\ \ \text{(by [10, eqs. (3.13)–(3.14)])}, \tag{2.15}$$

where

$$\Sigma_\theta=\{z\in\mathbb{C}:|\arg(z)|<\theta\}. \tag{2.16}$$

Since Δ generates a bounded analytic semigroup of angle $\frac{\pi}{2}$ on $L^2(\Omega)$, the properties (2.15) and (2.12) imply the following resolvent estimates (see [1, Theorem 3.7.11]):

$$\begin{aligned}\|(z^\alpha-\Delta)^{-1}\|&\leq c|z|^{-\alpha} && \forall\, z\in\Sigma_\theta,\ |\mathrm{Im}(z)|\leq\frac{\pi}{\tau},\\ \left\|\left(\left(\frac{1-e^{-\tau z}}{\tau}\right)^\alpha-\Delta\right)^{-1}\right\|&\leq c\left|\left(\frac{1-e^{-\tau z}}{\tau}\right)\right|^{-\alpha}\leq c|z|^{-\alpha} && \forall\, z\in\Sigma_\theta,\ |\mathrm{Im}(z)|\leq\frac{\pi}{\tau},\end{aligned} \tag{2.17}$$

where $\|\cdot\|$ denotes the operator norm on $L^2(\Omega)$.

We rewrite (2.4) into the following form:

$$\sum_{n=1}^\infty u_n\zeta^n=\left(\frac{1-\zeta}{\tau}\right)^{\alpha-1}\left(\left(\frac{1-\zeta}{\tau}\right)^\alpha-\Delta\right)^{-1}\frac{\zeta}{\tau}u_0. \tag{2.18}$$

For $\kappa>0$ and $\varrho_\kappa=e^{-(\kappa+1)\tau}\in(0,1)$, the Cauchy integral formula implies that

$$\begin{aligned}u_n&=\frac{1}{2\pi i}\int_{|\zeta|=\varrho_\kappa}\zeta^{-n-1}\sum_{m=1}^\infty u_m\zeta^m\mathrm{d}\zeta\\ &=\frac{1}{2\pi i}\int_{|\zeta|=\varrho_\kappa}\zeta^{-n}\left(\frac{1-\zeta}{\tau}\right)^{\alpha-1}\left(\left(\frac{1-\zeta}{\tau}\right)^\alpha-\Delta\right)^{-1}\frac{1}{\tau}u_0\mathrm{d}\zeta\\ &=\frac{1}{2\pi i}\int_{\Gamma^\tau}e^{t_nz}e^{-\tau z}\left(\frac{1-e^{-\tau z}}{\tau}\right)^{\alpha-1}\left(\left(\frac{1-e^{-\tau z}}{\tau}\right)^\alpha-\Delta\right)^{-1}u_0\,\mathrm{d}z,\end{aligned} \tag{2.19}$$

where the last equality is due to the change of variable $\zeta=e^{-z\tau}$ with the contour

$$\Gamma^\tau=\{z=\kappa+1+\mathrm{i}y:\ y\in\mathbb{R}\ \text{ and }\ |y|\leq\pi/\tau\}. \tag{2.20}$$

The angle condition (2.15) and [1, Theorem 3.7.11] imply that the integrand of (2.19) is analytic in the region

$$\Sigma_{\theta,\kappa}^\tau=\left\{z\in\mathbb{C}:|\arg(z)|\leq\theta,\ \ |z|\geq\kappa,\ |\mathrm{Im}(z)|\leq\frac{\pi}{\tau},\ \ \mathrm{Re}(z)\leq\kappa+1\right\}, \tag{2.21}$$

enclosed by the four paths Γ^τ, $\Gamma_{\theta,\kappa}^\tau$, and $\mathbb{R}\pm\mathrm{i}\pi/\tau$, where

$$\Gamma_{\theta,\kappa}^\tau=\{z\in\mathbb{C}:|z|=\kappa,|\arg z|\leq\theta\}\cup\left\{z\in\mathbb{C}:z=re^{\pm\mathrm{i}\theta},\kappa\leq r\leq\frac{\pi}{\tau\sin(\theta)}\right\}. \tag{2.22}$$

Then Cauchy's theorem allows us to deform the integration path from Γ^τ to $\Gamma^\tau_{\theta,\kappa}$ in the integral (2.19) (the integrals on $\mathbb{R} \pm \mathrm{i}\pi/\tau$ cancel each other). This yields the desired representation of the numerical solution

$$u_n = \frac{1}{2\pi i}\int_{\Gamma^\tau_{\theta,\kappa}} e^{t_n z} e^{-\tau z}\left(\frac{1-e^{-\tau z}}{\tau}\right)^{\alpha-1}\left(\left(\frac{1-e^{-\tau z}}{\tau}\right)^{\alpha} - \Delta\right)^{-1} u_0 \,\mathrm{d}z. \tag{2.23}$$

On the other hand, by using (2.3) and inverse Laplace transform, we have the following representation of the PDE's solution:

$$u(\cdot,t_n) = \frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}} e^{t_n z} z^{\alpha-1}(z^\alpha - \Delta)^{-1} u_0 \,\mathrm{d}z, \tag{2.24}$$

where

$$\Gamma_{\theta,\kappa} = \{z \in \mathbb{C} : |z| = \kappa, |\arg z| \le \theta\} \cup \left\{z \in \mathbb{C} : z = re^{\pm \mathrm{i}\theta}, \kappa \le r < \infty\right\}, \tag{2.25}$$

which differs from $\Gamma^\tau_{\theta,\kappa}$ by

$$\Gamma_{\theta,\kappa}\backslash\Gamma^\tau_{\theta,\kappa} = \left\{z \in \mathbb{C} : z = re^{\pm\mathrm{i}\theta}, \frac{\pi}{\tau\sin(\theta)} \le r < \infty\right\}. \tag{2.26}$$

It remains to compare (2.23) and (2.24) in order to make an estimate of the error $\|u_n - u(\cdot,t_n)\|_{L^2(\Omega)}$. To this end, we use (2.12)–(2.14) and (2.17) to estimate the difference between the integrands of (2.23) and (2.24):

$$\begin{aligned}
&\left\| e^{-\tau z}\left(\frac{1-e^{-\tau z}}{\tau}\right)^{\alpha-1}\left(\left(\frac{1-e^{-\tau z}}{\tau}\right)^{\alpha} - \Delta\right)^{-1} - z^{\alpha-1}(z^\alpha - \Delta)^{-1}\right\| \\
&= |e^{-\tau z}|\left\|\left(\frac{1-e^{-\tau z}}{\tau}\right)^{\alpha-1}\left(\left(\frac{1-e^{-\tau z}}{\tau}\right)^{\alpha} - \Delta\right)^{-1} - e^{\tau z} z^{\alpha-1}(z^\alpha - \Delta)^{-1}\right\| \\
&\le |e^{-\tau z}|\left\|\left(\left(\frac{1-e^{-\tau z}}{\tau}\right)^{\alpha} - z^\alpha\right)\left(\frac{1-e^{-\tau z}}{\tau}\right)^{-1}\left(\left(\frac{1-e^{-\tau z}}{\tau}\right)^{\alpha} - \Delta\right)^{-1}\right\| \\
&\quad + |e^{-\tau z}|\left\| z^\alpha\left(\left(\frac{1-e^{-\tau z}}{\tau}\right)^{-1} - z^{-1}\right)\left(\left(\frac{1-e^{-\tau z}}{\tau}\right)^{\alpha} - \Delta\right)^{-1}\right\| \\
&\quad + |e^{-\tau z}|\left\| z^{\alpha-1}\left[\left(\left(\frac{1-e^{-\tau z}}{\tau}\right)^{\alpha} - \Delta\right)^{-1} - \left(z^\alpha - \Delta\right)^{-1}\right]\right\| \\
&\quad + |e^{-\tau z}|\left\|(1-e^{\tau z}) z^{\alpha-1}\left(z^\alpha - \Delta\right)^{-1}\right\| \\
&=: |e^{-\tau z}|(I_1 + I_2 + I_3 + I_4),
\end{aligned} \tag{2.27}$$

where $|e^{-\tau z}| \le c$ for $z \in \Gamma^\tau_{\theta,\kappa}$ due to $\tau|z| \le c$, and $I_1 + I_2 \le c\tau$ for $z \in \Gamma^\tau_{\theta,\kappa}$, which is a simple consequence of (2.12)–(2.14) and (2.17). The two terms I_3 and I_4 are estimated below:

$$\begin{aligned}
I_3 &= |z|^{\alpha-1}\left\|\left(\left(\frac{1-e^{-\tau z}}{\tau}\right)^{\alpha} - \Delta\right)^{-1}\left(z^\alpha - \Delta\right)^{-1}\left(z^\alpha - \left(\frac{1-e^{-\tau z}}{\tau}\right)^{\alpha}\right)\right\| \le c\tau \\
&\qquad \forall\, z \in \Gamma^\tau_{\theta,\kappa}, \\
I_4 &= \left\|(1-e^{\tau z}) z^{\alpha-1}\left(z^\alpha - \Delta\right)^{-1}\right\| \le c\tau,
\end{aligned}$$

where the last two inequalities are also simple consequences of (2.12)–(2.14) and (2.17). Substituting the estimates of I_1, I_2, I_3, and I_4 into (2.27), we obtain

(2.28)
$$\left\| e^{-\tau z}\left(\frac{1-e^{-\tau z}}{\tau}\right)^{\alpha-1}\left(\left(\frac{1-e^{-\tau z}}{\tau}\right)^{\alpha}-\Delta\right)^{-1} - z^{\alpha-1}(z^\alpha-\Delta)^{-1}\right\| \le c\tau \quad \forall\, z\in\Gamma^\tau_{\theta,\kappa}.$$

Then the difference between (2.23) and (2.24) yields

$$\begin{aligned}
&\|u_n(x)-u(\cdot,t_n)\|_{L^2(\Omega)}\\
&\le c\int_{\Gamma^\tau_{\theta,\kappa}} e^{\mathrm{Re}(z)t_n}\left\| e^{-\tau z}\left(\frac{1-e^{-\tau z}}{\tau}\right)^{\alpha-1}\left(\left(\frac{1-e^{-\tau z}}{\tau}\right)^{\alpha}-\Delta\right)^{-1} - z^{\alpha-1}(z^\alpha-\Delta)^{-1}\right\| \|u_0\|_{L^2(\Omega)}|\mathrm{d}z|\\
&\quad + c\int_{\Gamma_{\theta,\kappa}\setminus\Gamma^\tau_{\theta,\kappa}} e^{\mathrm{Re}(z)t_n}\left\|z^{\alpha-1}(z^\alpha-\Delta)^{-1}\right\|\|u_0\|_{L^2(\Omega)}|\mathrm{d}z|\\
&\le c\int_{\Gamma^\tau_{\theta,\kappa}} e^{\mathrm{Re}(z)t_n}\tau|\mathrm{d}z| + c\int_{\Gamma_{\theta,\kappa}\setminus\Gamma^\tau_{\theta,\kappa}} e^{\mathrm{Re}(z)t_n}|z|^{-1}|\mathrm{d}z| \qquad \text{(use (2.28) and (2.17) here)}\\
&\le \left(c\int_\kappa^{\frac{\pi}{\tau\sin(\theta)}} e^{r\cos(\theta)t_n}\tau\mathrm{d}r + c\int_{-\theta}^{\theta} e^{\kappa\cos(\varphi)t_n}\tau\kappa\mathrm{d}\varphi\right) + c\int_{\frac{\pi}{\tau\sin(\theta)}}^\infty e^{r\cos(\theta)t_n} r^{-1}\mathrm{d}r,
\end{aligned}$$
(2.29)

where we have used (2.22) and (2.26) in the last inequality. By using the change of variable $s=rt_n$ and noting that $\cos(\theta)<0$ for $\theta\in(\frac{\pi}{2},\pi)$, we have

$$\int_\kappa^{\frac{\pi}{\tau\sin(\theta)}} e^{r\cos(\theta)t_n}\tau\mathrm{d}r = t_n^{-1}\tau\int_{\kappa t_n}^{\frac{\pi t_n}{\tau\sin(\theta)}} e^{-s|\cos(\theta)|}\mathrm{d}s \le ct_n^{-1}\tau \tag{2.30}$$

and

$$\begin{aligned}
\int_{\frac{\pi}{\tau\sin(\theta)}}^\infty e^{r\cos(\theta)t_n}r^{-1}\mathrm{d}r &\le \left(\frac{\pi}{\tau\sin(\theta)}\right)^{-1}\int_{\frac{\pi}{\tau\sin(\theta)}}^\infty e^{-r|\cos(\theta)|t_n}\mathrm{d}r\\
&= t_n^{-1}\left(\frac{\pi}{\tau\sin(\theta)}\right)^{-1}\int_{\frac{\pi t_n}{\tau\sin(\theta)}}^\infty e^{-s|\cos(\theta)|}\mathrm{d}s \le ct_n^{-1}\tau.
\end{aligned} \tag{2.31}$$

Substituting the last two estimates into (2.29) yields

$$\|u_n-u(\cdot,t_n)\|_{L^2(\Omega)} \le \left(ct_n^{-1}\tau + c\kappa e^{\kappa t_n}\tau\right) + ct_n^{-1}\tau \le c(\kappa e^{\kappa T}+t_n^{-1})\tau. \tag{2.32}$$

3. Application of the methodology to (1.5). In this section, we apply the method of analysis described in the last section to the tempered fractional Feynman–Kac equation (1.5), and point out the main differences. The technical proofs are deferred to section 4.

3.1. Inverse Laplace transform representation of the solution. Similarly to section 2.1, we consider the Laplace transform of (1.5), namely,

$$\begin{aligned}
&(z+\lambda-ipU(x))\widehat{G}(x,z) - G_0(x) - \big(\lambda^\alpha+\Delta\big)(z+\lambda-ipU(x))^{1-\alpha}\widehat{G}(x,z)\\
&\quad = -G_0(x)(\lambda^\alpha(z+\lambda-ipU(x))^{1-\alpha}-\lambda)(z-ipU(x))^{-1},
\end{aligned} \tag{3.1}$$

where $\widehat{G}(x,z)=\int_0^\infty G(x,t)e^{-tz}\mathrm{d}t$ denotes the Laplace transform of $G(x,t)$ in time. By introducing the notations

$$\eta(x,z)=(z+\lambda-ipU(x))^\alpha-\lambda^\alpha,\quad \beta(x,z)=z+\lambda-ipU(x) \tag{3.2}$$

with the abbreviations

$$\eta(z)=\eta(\cdot,z),\quad \beta(z)=\beta(\cdot,z), \tag{3.3}$$

we reformulate (3.1) in the following way, collecting all the terms involving $G_0(x)$ to the right-hand side of the equation:

$$\big(\eta(z)-\Delta\big)\beta(z)^{1-\alpha}\widehat{G}(x,z)=G_0(x)\beta(z)^{1-\alpha}\frac{\eta(z)}{z-ipU(x)}. \tag{3.4}$$

From (3.4) we derive

$$\widehat{G}(x,z)=\beta(z)^{\alpha-1}\big(\eta(z)-\Delta\big)^{-1}\left(\beta(z)^{1-\alpha}\frac{G_0(x)\eta(z)}{z-ipU(x)}\right). \tag{3.5}$$

Due to the noncommutativity between $(\eta(z)-\Delta)^{-1}$ and $\beta(z)^{1-\alpha}$, the two terms $\beta(z)^{\alpha-1}$ and $\beta(z)^{1-\alpha}$ in the expression above cannot be canceled. By using the inverse Laplace transform, we have

$$G(x,t)=\frac{1}{2\pi i}\int_{\kappa+1+i\mathbb{R}}e^{tz}\beta(z)^{\alpha-1}\big(\eta(z)-\Delta\big)^{-1}\left(\beta(z)^{1-\alpha}\frac{G_0(x)\eta(z)}{z-ipU(x)}\right)\mathrm{d}z. \tag{3.6}$$

From Proposition 3.1 below we see that the integrand in (3.6) is an $M(\Omega)$-valued analytic function for $z\in\Sigma_{\theta,\kappa}^\tau$ (see (2.21) for the definition of $\Sigma_{\theta,\kappa}^\tau$). Consequently, similarly to the last section (cf. (2.19)–(2.23)), we can deform the integration path from $\kappa+1+i\mathbb{R}$ to $\Gamma_{\theta,\kappa}$ (defined in (2.25)):

$$G(x,t)=\frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}}e^{tz}\beta(z)^{\alpha-1}\big(\eta(z)-\Delta\big)^{-1}\left(\beta(z)^{1-\alpha}\frac{G_0(x)\eta(z)}{z-ipU(x)}\right)\mathrm{d}z. \tag{3.7}$$

This integral representation will be used for estimating the error of the numerical solutions.

PROPOSITION 3.1. *By choosing $\theta\in(\frac{\pi}{2},\pi)$ sufficiently close to $\frac{\pi}{2}$ and $\kappa>0$ sufficiently large (depending on the value $\lambda+|p|\|U\|_{C(\overline{\Omega})}$), we have the following results:*

(1) *For all $x\in\Omega$ and $z\in\Sigma_{\theta,\kappa}$, we have $\beta(z)\in\Sigma_{\frac{3\pi}{4},\frac{\kappa}{2}}$ and $\eta(z)\in\Sigma_{\frac{3\pi}{4},\frac{\kappa^\alpha}{2}}$, and*

$$c|z|\le|\beta(z)|\le c|z|,\qquad c|z|^\alpha\le|\eta(z)|\le c|z|^\alpha, \tag{3.8}$$

where

$$\Sigma_{\theta,\kappa}=\{z\in\mathbb{C}:|z|\ge\kappa,|\arg(z)|\le\theta\}. \tag{3.9}$$

Consequently, $\beta(z)^{1-\alpha}$, $\beta(z)^{\alpha-1}$, and $\eta(z)$ are all $C(\overline{\Omega})$-valued analytic function of $z\in\Sigma_{\theta,\kappa}$.

(2) *The operator $\big(\eta(z)-\Delta\big)^{-1}:M(\Omega)\to M(\Omega)$ is well-defined, bounded, and analytic with respect to $z\in\Sigma_{\theta,\kappa}$, satisfying*

$$\big\|\Delta\big(\eta(z)-\Delta\big)^{-1}\big\|_{M(\Omega)\to M(\Omega)}\le c\qquad\forall\, z\in\Sigma_{\theta,\kappa}, \tag{3.10}$$

$$\big\|\big(\eta(z)-\Delta\big)^{-1}\big\|_{M(\Omega)\to M(\Omega)}\le c|z|^{-\alpha}\qquad\forall\, z\in\Sigma_{\theta,\kappa}. \tag{3.11}$$

(3) *The contour integral* (3.7) *defines a solution of* (1.5) *under the initial and boundary conditions* (1.8), (1.9), *with the regularity* $G(\cdot,t) \in M(\Omega)$, $D_t G(\cdot,t) \in M(\Omega)$, $D_t^{1-\alpha} G(\cdot,t) \in M(\Omega)$, *and* $\Delta D_t^{1-\alpha} G(\cdot,t) \in M(\Omega)$ *for* $t \in (0,T]$. *The solution given by* (3.7) *is called the mild solution of* (1.5), *with each term of* (1.5) *well-defined as a measure.*

The proof of Proposition 3.1 is presented in section 4.1, which is the main difference between this subsection and the derivation of (2.24) in section 2. In the following two subsections, we present a numerical method for approximating the mild solution of (1.5) given by (3.6).

3.2. Discretization of the fractional substantial derivative. By straightforward calculation, we see that the fractional substantial derivative $D_t(x)^{1-\alpha}$ defined in (1.6) has the following decomposition:

$$\begin{aligned} &D_t(x)^{1-\alpha} G(x,t) \\ &\quad = \frac{1}{\Gamma(\alpha)}\left(\lambda - ipU(x) + \frac{\partial}{\partial t}\right)\left(e^{-t(\lambda - ipU(x))}\int_0^t \frac{1}{(t-s)^{1-\alpha}} e^{s(\lambda-ipU(x))} G(x,s)\mathrm{d}s\right) \\ &\quad = e^{-t(\lambda-ipU(x))}\frac{1}{\Gamma(\alpha)}\frac{\partial}{\partial t}\int_0^t \frac{1}{(t-s)^{1-\alpha}} e^{s(\lambda-ipU(x))} G(x,s)\mathrm{d}s \\ &\quad = e^{-t(\lambda-ipU(x))}\partial_t^{1-\alpha}\big(e^{t(\lambda-ipU(x))}G(x,t)\big), \end{aligned} \tag{3.12}$$

where $\partial_t^{1-\alpha}$ is the standard Riemann–Liouville fractional derivative defined in (1.3). In view of (3.12), we approximate the fractional substantial derivative $D_t(x)^{1-\alpha} G(x,t_n)$ by

$$\overline{D_\tau}(x)^{1-\alpha} G_n(x) := e^{-t_n(\lambda-ipU(x))}\overline{\partial_\tau}^{1-\alpha}\big(e^{t_n(\lambda-ipU(x))}G_n(x)\big), \tag{3.13}$$

which relates the discretized fractional substantial derivative $\overline{D_\tau}(x)^{1-\alpha}$ to the standard backward Euler convolution quadrature defined in (2.6).

Consistent with the notation $\overline{D_\tau}(x)^{1-\alpha}$ introduced above, we denote by $\overline{D_\tau}(x)$ the time discretization of the differential operator $D_t(x)$, defined by

$$\begin{aligned} \overline{D_\tau}(x) G_n(x) &= e^{-t_n(\lambda-ipU(x))}\overline{\partial_\tau}\big(e^{t_n(\lambda-ipU(x))}G_n(x)\big) \\ &= e^{-t_n(\lambda-ipU(x))}\frac{e^{t_n(\lambda-ipU(x))}G_n(x) - e^{t_{n-1}(\lambda-ipU(x))}G_{n-1}(x)}{\tau}. \end{aligned} \tag{3.14}$$

With the notation (3.13), we have

$$\begin{aligned} &\sum_{n=1}^{\infty} \overline{D_\tau}^{1-\alpha}(x) G_n(x)\zeta^n \\ &\quad = \sum_{n=1}^{\infty} \overline{\partial_\tau}^{1-\alpha}\big(e^{t_n(\lambda-ipU(x))}G_n(x)\big)(e^{-\tau(\lambda-ipU(x))}\zeta)^n \\ &\quad = \left(\frac{1-e^{-\tau(\lambda-ipU(x))}\zeta}{\tau}\right)^{1-\alpha}\sum_{n=1}^{\infty}\big(e^{t_n(\lambda-ipU(x))}G_n(x)\big)(\zeta e^{-\tau(\lambda-ipU(x))})^n \\ &\quad = \left(\frac{1-e^{-\tau(\lambda-ipU(x))}\zeta}{\tau}\right)^{1-\alpha}\sum_{n=1}^{\infty} G_n(x)\zeta^n. \end{aligned} \tag{3.15}$$

The identity (3.15) motivates our approximation of (3.4) in the next subsection.

3.3. Derivation of the time-stepping scheme. Let $\eta_\tau(x,z)$ and $\beta_\tau(x,z)$ be approximations of $\eta(x,z)$ and $\beta(x,z)$, respectively, defined by

$$\eta_\tau(x,z) = \left(\frac{1-e^{-\tau(z+\lambda-ipU(x))}}{\tau}\right)^\alpha - \lambda^\alpha, \quad \beta_\tau(x,z) = \frac{1-e^{-\tau(z+\lambda-ipU(x))}}{\tau} \tag{3.16}$$

with the abbreviations

$$\eta_\tau(z) = \eta_\tau(\cdot,z), \quad \beta_\tau(z) = \beta_\tau(\cdot,z), \tag{3.17}$$

and choose $\frac{\tau e^{-\tau(z-ipU(x))}}{1-e^{-\tau(z-ipU(x))}}$ to be the approximation of $\frac{1}{z-ipU(x)}$ in (3.4). Analogous to the last section, we start with approximating the problem on the Laplace transform side. In other words, we wish to construct the numerical solutions $G_n(x)$, $n=1,2,\ldots,$ satisfying the equation

$$\begin{aligned}&\big(\eta_\tau(z)-\Delta\big)\beta_\tau(z)^{1-\alpha}\tau\sum_{n=1}^{\infty}G_n(x)e^{-t_nz}\\ &\quad= G_0(x)\beta_\tau(z)^{1-\alpha}\eta_\tau(z)\frac{\tau e^{-\tau(z-ipU(x))}}{1-e^{-\tau(z-ipU(x))}},\end{aligned} \tag{3.18}$$

where $\tau\sum_{n=1}^{\infty}G_n(x)e^{-t_nz}$ approximates the Laplace transform $\widehat{G}(x,z)$ in (3.4). To this end, it suffices to construct $G_n(x)$, $n=1,2,\ldots,$ satisfying the following equation (replacing $e^{-\tau z}$ by the notation ζ in the last equation):

$$\begin{aligned}&\left(\left(\frac{1-e^{-\tau(\lambda-ipU(x))}\zeta}{\tau}\right)^\alpha-\lambda^\alpha-\Delta\right)\left(\frac{1-e^{-\tau(\lambda-ipU(x))}\zeta}{\tau}\right)^{1-\alpha}\sum_{n=1}^{\infty}G_n(x)\zeta^n\\ &\quad= G_0(x)\left(\frac{1-e^{-\tau(\lambda-ipU(x))}\zeta}{\tau}\right)^{1-\alpha}\left(\left(\frac{1-e^{-\tau(\lambda-ipU(x))}\zeta}{\tau}\right)^\alpha-\lambda^\alpha\right)\frac{e^{i\tau pU(x)}\zeta}{1-e^{i\tau pU(x)}\zeta}.\end{aligned} \tag{3.19}$$

In view of (3.15), the last equation is equivalent to

$$\begin{aligned}&\sum_{n=1}^{\infty}\left(\big(\overline{D_\tau}(x)^\alpha-\lambda^\alpha-\Delta\big)\overline{D_\tau}(x)^{1-\alpha}G_n(x)\right)\zeta^n\\ &\quad=\sum_{n=1}^{\infty}\left(G_0(x)\overline{D_\tau}(x)^{1-\alpha}\big(\overline{D_\tau}(x)^\alpha-\lambda^\alpha\big)e^{ipU(x)t_n}\right)\zeta^n.\end{aligned} \tag{3.20}$$

Consequently, we define $G_n(x)$, $n=1,2,\ldots,$ to be the solutions of

$$\begin{aligned}&\big(\overline{D_\tau}(x)^\alpha-\lambda^\alpha-\Delta\big)\overline{D_\tau}(x)^{1-\alpha}G_n(x)\\ &\qquad= G_0(x)\overline{D_\tau}(x)^{1-\alpha}\big(\overline{D_\tau}(x)^\alpha-\lambda^\alpha\big)e^{ipU(x)t_n}.\end{aligned} \tag{3.21}$$

Similar to the product rule (2.9), it is straightforward to verify the following identity:

$$\overline{D_\tau}(x)^\alpha\overline{D_\tau}(x)^{1-\alpha}G_n(x) = \begin{cases}\dfrac{1}{\tau}G_1(x) & \text{if } n=1,\\ \overline{D_\tau}(x)G_n(x) & \text{if } 2\le n\le N.\end{cases} \tag{3.22}$$

By using (3.22), the numerical scheme (3.21) can be equivalently written as

$$\begin{aligned}&\big(\overline{D_\tau}(x) - (\lambda^\alpha + \Delta)\overline{D_\tau}(x)^{1-\alpha}\big)G_n(x)\\&\quad = G_0(x)\big(\overline{D_\tau}(x) - \lambda^\alpha\overline{D_\tau}(x)^{1-\alpha}\big)e^{ipU(x)t_n}\\&\quad = -G_0(x)\left(\lambda^\alpha\overline{D_\tau}(x)^{1-\alpha} - \frac{1-e^{-\lambda\tau}}{\tau}\right)e^{ipU(x)t_n}, \qquad n = 1, 2, \ldots, N.\end{aligned} \tag{3.23}$$

The scheme (3.23) is equivalent to applying the implicit Euler scheme to the equation

$$\begin{aligned}&D_t(x)G(x,t) - (\lambda^\alpha + \Delta)D_t(x)^{1-\alpha}G(x,t)\\&\qquad\qquad = -G_0(x)\left(\lambda^\alpha D_t(x)^{1-\alpha} - \frac{1-e^{-\lambda\tau}}{\tau}\right)e^{ipU(x)t},\end{aligned} \tag{3.24}$$

which replaces a constant λ in the original equation (1.5) by $\frac{1-e^{-\lambda\tau}}{\tau}$.

Remark 3.1. The evaluation of the discrete convolutions in (3.23) is computationally expensive whereas some fast algorithms can be applied. The fast algorithm developed in [11] can be used to evaluate the discrete convolutions exactly with $\mathcal{O}(\log^2 N)$ operations and $\mathcal{O}(N)$ storage (up to the Nth time step). Instead of evaluating the discrete convolutions exactly, one can also approximate the discrete convolutions with error ϵ (see, for example, [2, 34]), with complexity $\mathcal{O}(N(\log N)\log\frac{1}{\epsilon})$ and storage $\mathcal{O}((\log N)\log\frac{1}{\epsilon})$.

In the next subsection, we estimate the error of the numerical solution given by (3.23) by using the identity (3.18).

3.4. Error estimate for the time-stepping scheme (3.23). Applying Cauchy's integral formula yields, for $\varrho_\kappa = e^{-\tau(\kappa+1)} \in (0,1)$,

$$G_n(x) = \frac{1}{2\pi \mathrm{i}}\int_{|\zeta|=\varrho_\kappa}\zeta^{-n-1}\sum_{m=1}^{\infty}G_m(x)\zeta^m\,d\zeta = \frac{1}{2\pi\mathrm{i}}\int_{\Gamma^\tau}e^{zt_n}\left(\sum_{n=1}^{\infty}G_n(x)e^{-t_nz}\right)\tau\,dz, \tag{3.25}$$

where the second equality is due to the change of variable $\zeta = e^{-z\tau}$ with the contour Γ^τ defined in (2.20). From (3.18) we see that

$$\sum_{n=1}^{\infty}G_n(x)e^{-t_nz} = \beta_\tau(z)^{\alpha-1}\big(\eta_\tau(z)-\Delta\big)^{-1}\left(G_0(x)\beta_\tau(z)^{1-\alpha}\frac{\eta_\tau(z)e^{-\tau(z-ipU(x))}}{1-e^{-\tau(z-ipU(x))}}\right), \tag{3.26}$$

which together with (3.25) gives

$$\begin{aligned}G_n(x) &= \frac{1}{2\pi\mathrm{i}}\int_{\Gamma^\tau}e^{zt_n}\beta_\tau(z)^{\alpha-1}\big(\eta_\tau(z)-\Delta\big)^{-1}\left(G_0(x)\beta_\tau(z)^{1-\alpha}\frac{\eta_\tau(z)\tau e^{-\tau(z-ipU(x))}}{1-e^{-\tau(z-ipU(x))}}\right)dz\\&= \frac{1}{2\pi\mathrm{i}}\int_{\Gamma^\tau_{\theta,\kappa}}e^{zt_n}\beta_\tau(z)^{\alpha-1}\big(\eta_\tau(z)-\Delta\big)^{-1}\left(G_0(x)\beta_\tau(z)^{1-\alpha}\frac{\eta_\tau(z)\tau e^{-\tau(z-ipU(x))}}{1-e^{-\tau(z-ipU(x))}}\right)dz,\end{aligned} \tag{3.27}$$

where we have deformed the integration path (using Cauchy's theorem of complex analysis) from Γ^τ to $\Gamma^\tau_{\theta,\kappa}$ defined in (2.22). Such a deformation requires the integrand in (3.6) to be an $M(\Omega)$-valued analytic function for $z \in \Sigma^\tau_{\theta,\kappa}$ (see (2.21) for the definition of $\Sigma_{\theta,\kappa}^\tau$), which is a consequence of Proposition 3.2 below. Unlike the analysis of (1.1), where the integrand of (2.23) is clearly analytic in the region $\Sigma_{\theta,\kappa}^\tau$ due to property (2.15). The proof of Proposition 3.2 is more technical and presented in section 4.2.

PROPOSITION 3.2. *By choosing $\theta \in (\frac{\pi}{2}, \pi)$ sufficiently close to $\frac{\pi}{2}$ and $\kappa > 0$ sufficiently large (depending on $\lambda + |p|\|U\|_{C(\overline{\Omega})}$), there exists a positive constant τ_* (depending on θ and κ) such that the following estimates hold when $\tau \le \tau_*$:*

(1′) *$\beta_\tau(z), \eta_\tau(z) \in \Sigma_{\frac{3\pi}{4}}$ for $z \in \Sigma_{\theta,\kappa}^\tau$, and*

$$c|z| \le |\beta_\tau(z)| \le c|z|, \qquad c|z|^\alpha \le |\eta_\tau(z)| \le c|z|^\alpha \qquad \forall\, z \in \Sigma_{\theta,\kappa}^\tau. \tag{3.28}$$

(2′) *The operator $(\eta_\tau(z) - \Delta)^{-1}$ is bounded and analytic in $M(\Omega)$ for $z \in \Sigma_{\theta,\kappa}^\tau$, satisfying*

$$\left\| \left(\eta_\tau(z) - \Delta\right)^{-1} \right\|_{M(\Omega)\to M(\Omega)} \le c|z|^{-\alpha} \quad \forall\, z \in \Sigma_{\theta,\kappa}^\tau.$$

By using the integral representations (3.7) and (3.27) derived in the last two sections, as well as Propositions 3.1 and 3.2, we prove the convergence of the discrete solutions given by (3.23). The result is presented in the following theorem.

THEOREM 3.3. *There exists a positive constant τ_* (see Proposition 3.2) such that for $\tau \le \tau_*$, the solution of (1.5) under the initial and boundary conditions (1.8)–(1.9) and the solution of (3.23) satisfy the following error estimate:*

$$\|G(\cdot, t_n) - G_n\|_{M(\Omega)} \le c_T \|G_0\|_{M(\Omega)}\, t_n^{-1}\tau, \qquad n = 1, 2, \ldots, N, \tag{3.29}$$

where the constant c_T may grow exponentially with respect to T and the quantity $\lambda + |p|\|U\|_{C(\overline{\Omega})}$.

Remark 3.2. The factor t_n^{-1} in the error estimate is sharp (cf. [21, estimate (1.14)]). One cannot expect any uniform accuracy up to time $t = 0$, due to the possible nonsmoothness of the initial data G_0, which is only assumed to be a measure on Ω (such as the Delta function).

Proof of Theorem 3.3. Consider the difference between (3.7) and (3.27):

$$\begin{aligned}
&G(x, t_n) - G_n(x)\\
&\quad = \frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}\backslash\Gamma_{\theta,\kappa}^\tau} e^{t_n z}\beta(z)^{\alpha-1}\big(\eta(z)-\Delta\big)^{-1}\left(\beta(z)^{1-\alpha}\frac{G_0(x)\eta(z)}{z - ipU(x)}\right)\mathrm{d}z\\
&\qquad + \frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}^\tau} e^{t_n z}\Bigg[\beta(z)^{\alpha-1}\big(\eta(z)-\Delta\big)^{-1}\left(\beta(z)^{1-\alpha}\frac{G_0(x)\eta(z)}{z - ipU(x)}\right)\\
&\qquad\qquad - \beta_\tau(z)^{\alpha-1}\big(\eta_\tau(z)-\Delta\big)^{-1}\\
&\qquad\qquad \left(\beta_\tau(z)^{1-\alpha}\frac{G_0(x)\eta_\tau(z)\tau e^{-\tau(z-ipU(x))}}{1-e^{-\tau(z-ipU(x))}}\right)\Bigg]\mathrm{d}z\\
&\quad =: J_1 + J_2.
\end{aligned}\tag{3.30}$$

Note that $|z - ipU(x)| \ge \frac{1}{2}|z|$ on the contour $\Gamma_{\theta,\kappa}$, due to the largeness of κ compared with $\lambda + |p|\|U\|_{C(\overline{\Omega})}$. By denoting $|\mathrm{d}z|$ to be the arc length element on the contour $\Gamma_{\theta,\kappa}\backslash\Gamma_{\theta,\kappa}^\tau$, we have

$$\|J_1\|_{M(\Omega)} \le c\int_{\Gamma_{\theta,\kappa}\backslash\Gamma_{\theta,\kappa}^\tau} e^{t_n|z|\cos(\theta)}\left\|\beta(z)^{\alpha-1}\big(\eta(z)-\Delta\big)^{-1}\left(\beta(z)^{1-\alpha}\frac{G_0\eta(z)}{z-ipU(x)}\right)\right\|_{M(\Omega)}|\mathrm{d}z|,$$

where

$$
\begin{aligned}
&\left\|\beta(z)^{\alpha-1}\big(\eta(z)-\Delta\big)^{-1}\left(\beta(z)^{1-\alpha}\frac{G_0\eta(z)}{z-ipU(x)}\right)\right\|_{M(\Omega)} \\
&\quad\le c\|\beta(z)^{\alpha-1}\|_{C(\overline{\Omega})}\|\big(\eta(z)-\Delta\big)^{-1}\|_{M(\Omega)\to M(\Omega)}\left\|\beta(z)^{1-\alpha}\frac{G_0\eta(z)}{z-ipU(x)}\right\|_{M(\Omega)} \\
&\quad\le c\|\beta(z)\|_{C(\overline{\Omega})}^{\alpha-1}\|\big(\eta(z)-\Delta\big)^{-1}\|_{M(\Omega)\to M(\Omega)}\|\beta(z)\|_{C(\overline{\Omega})}^{1-\alpha}\left\|\frac{\eta(z)}{z-ipU(x)}\right\|_{C(\overline{\Omega})}\|G_0\|_{M(\Omega)} \\
&\quad\le c|z|^{\alpha-1}|z|^{-\alpha}|z|^{1-\alpha}|z|^{\alpha-1}\|G_0\|_{M(\Omega)} \\
&\qquad\text{(use (3.8), (3.11) and } |z-ipU(x)|\ge \tfrac12|z| \text{ on } \Gamma_{\theta,\kappa}\backslash\Gamma_{\theta,\kappa}^{\tau}) \\
&\quad\le c|z|^{-1}\|G_0\|_{M(\Omega)}.
\end{aligned}
$$

Consequently, we obtain

$$
\begin{aligned}
\|J_1\|_{M(\Omega)} &\le c\|G_0\|_{M(\Omega)}\int_{\Gamma_{\theta,\kappa}\backslash\Gamma_{\theta,\kappa}^{\tau}} e^{t_n|z|\cos(\theta)}|z|^{-1}\,|\mathrm{d}z| \\
&= c\|G_0\|_{M(\Omega)}\int_{\frac{\pi}{\tau\sin(\theta)}}^{\infty} e^{t_n r\cos(\theta)}r^{-1}\,\mathrm{d}r \qquad \text{(use (2.26))} \\
&\le c\|G_0\|_{M(\Omega)}\int_{\frac{\pi t_n}{\tau\sin(\theta)}}^{\infty} e^{s\cos(\theta)}s^{-1}\,\mathrm{d}s \qquad \text{(use the change of variable } s=t_n r) \\
&\le c\|G_0\|_{M(\Omega)}\frac{\tau\sin(\theta)}{\pi t_n}\int_{\frac{\pi t_n}{\tau\sin(\theta)}}^{\infty} e^{s\cos(\theta)}\mathrm{d}s \le c\|G_0\|_{M(\Omega)}t_n^{-1}\tau.
\end{aligned}
$$

In order to estimate $\|J_2\|_{M(\Omega)}$ in (3.30) we need to use the following lemma, whose proof is deferred to the next subsection.

LEMMA 3.4.

$$
\begin{aligned}
&\left\|\beta(z)^{\alpha-1}\big(\eta(z)-\Delta\big)^{-1}\left(\beta(z)^{1-\alpha}\frac{G_0\eta(z)}{z-ipU}\right)\right. \\
&\qquad\left. -\beta_\tau(z)^{\alpha-1}\big(\eta_\tau(z)-\Delta\big)^{-1}\left(\beta_\tau(z)^{1-\alpha}\frac{G_0\eta_\tau(z)\tau e^{-\tau(z-ipU)}}{1-e^{-\tau(z-ipU)}}\right)\right\|_{M(\Omega)} \\
&\le c\|G_0\|_{M(\Omega)}\tau \qquad \forall\, z\in\Gamma_{\theta,\kappa}^{\tau}.
\end{aligned}
\tag{3.31}
$$

By using Lemma 3.4, we have

$$
\begin{aligned}
\|J_2\|_{M(\Omega)} &\le c\|G_0\|_{M(\Omega)}\tau\int_{\Gamma_{\theta,\kappa}^{\tau}} e^{t_n|z|\cos(\arg(z))}|\mathrm{d}z| \\
&\le c\|G_0\|_{M(\Omega)}\tau\int_{\kappa}^{\frac{\pi}{\tau\sin(\theta)}} e^{t_n r\cos(\theta)}\mathrm{d}r + c\|G_0\|_{M(\Omega)}\tau\int_{-\theta}^{\theta} e^{t_n\kappa\cos(\varphi)}\kappa\mathrm{d}\varphi \\
&\le c\|G_0\|_{M(\Omega)}t_n^{-1}\tau\int_{\kappa t_n}^{\frac{\pi t_n}{\tau\sin(\theta)}} e^{s\cos(\theta)}\mathrm{d}s + c\|G_0\|_{M(\Omega)}\tau\kappa\int_{-\theta}^{\theta} e^{T\kappa}\mathrm{d}\varphi \\
&\le c\|G_0\|_{M(\Omega)}(t_n^{-1}+\kappa e^{\kappa T})\tau \\
&\le c_T\|G_0\|_{M(\Omega)}t_n^{-1}\tau \qquad \text{(note that } \kappa e^{\kappa T}\le \kappa T e^{\kappa T}t_n^{-1}).
\end{aligned}
\tag{3.32}
$$

This completes the proof of Theorem 3.3 in view of (3.30). ∎

3.5. Proof of Lemma 3.4. In this subsection we prove Lemma 3.4, which is used in the proof of Theorem 3.3 in the last subsection. To this end, we note that

$$
\begin{aligned}
&\Big\|\beta(z)^{\alpha-1}\big(\eta(z)-\Delta\big)^{-1}\Big(\beta(z)^{1-\alpha}\frac{G_0\eta(z)}{z-ipU}\Big)\\
&\quad-\beta_\tau(z)^{\alpha-1}\big(\eta_\tau(z)-\Delta\big)^{-1}\Big(\beta_\tau(z)^{1-\alpha}\frac{G_0\eta_\tau(z)\tau e^{-\tau(z-ipU)}}{1-e^{-\tau(z-ipU)}}\Big)\Big\|_{M(\Omega)}\\
&\le\Big\|\big(\beta(z)^{\alpha-1}-\beta_\tau(z)^{\alpha-1}\big)\big(\eta(z)-\Delta\big)^{-1}\Big(\beta(z)^{1-\alpha}\frac{G_0\eta(z)}{z-ipU}\Big)\Big\|_{M(\Omega)}\\
&\quad+\Big\|\beta_\tau(z)^{\alpha-1}\big((\eta(z)-\Delta)^{-1}-(\eta_\tau(z)-\Delta)^{-1}\big)\Big(\beta(z)^{1-\alpha}\frac{G_0\eta(z)}{z-ipU}\Big)\Big\|_{M(\Omega)}\\
&\quad+\Big\|\beta_\tau(z)^{\alpha-1}(\eta_\tau(z)-\Delta)^{-1}\Big((\beta(z)^{1-\alpha}-\beta_\tau(z)^{1-\alpha})\frac{G_0\eta(z)}{z-ipU}\Big)\Big\|_{M(\Omega)}\\
&\quad+\Big\|\beta_\tau(z)^{\alpha-1}(\eta_\tau(z)-\Delta)^{-1}\Big(\beta_\tau(z)^{1-\alpha}\frac{G_0(\eta(z)-\eta_\tau(z))}{z-ipU}\Big)\Big\|_{M(\Omega)}\\
&\quad+\Big\|\beta_\tau(z)^{\alpha-1}(\eta_\tau(z)-\Delta)^{-1}\Big(\beta_\tau(z)^{1-\alpha}G_0\eta_\tau(z)\Big(\frac{1}{z-ipU}-\frac{\tau e^{-\tau(z-ipU)}}{1-e^{-\tau(z-ipU)}}\Big)\Big)\Big\|_{M(\Omega)}\\
&\quad=:I_1^*+I_2^*+I_3^*+I_4^*+I_5^*.
\end{aligned}
\tag{3.33}
$$

To estimate $\beta(z)^{\alpha-1}-\beta_\tau(z)^{\alpha-1}$ in I_1 and $\beta(z)^{1-\alpha}-\beta_\tau(z)^{1-\alpha}$ in I_3, we denote $w=z+\lambda-ipU(x)$ and use the Taylor expansion

$$e^{-\tau w}=1-\tau w+\frac{1}{2}\tau^2w^2\int_0^1 e^{-\theta\tau w}(1-\theta)\mathrm{d}\theta.$$

Then we have

$$
\begin{aligned}
|\beta(z)^\gamma-\beta_\tau(z)^\gamma|&=\Big|\beta(z)^\gamma-\Big(\frac{1-e^{-\tau\beta(z)}}{\tau}\Big)^\gamma\Big|\\
&=\Big|\beta(z)^\gamma-\Big(\beta(z)-\tau\beta(z)^2\int_0^1 e^{-\theta\tau\beta(z)}(1-\theta)\mathrm{d}\theta\Big)^\gamma\Big|\\
&=|\beta(z)|^\gamma\Big|1-\Big(1-\tau\beta(z)\int_0^1 e^{-\theta\tau\beta(z)}(1-\theta)\mathrm{d}\theta\Big)^\gamma\Big|.
\end{aligned}
$$

If $\tau|\beta(z)|<\frac{1}{2}$, then the following Taylor expansion holds:

$$\Big(1-\frac{1}{2}\tau\beta(z)\int_0^1 e^{-\theta\tau w}(1-\theta)\mathrm{d}\theta\Big)^\gamma=1+O\big(\tau\beta(z)\textstyle\int_0^1 e^{-\theta\tau w}(1-\theta)\mathrm{d}\theta\big)=1+O(\tau|\beta(z)|).$$

In this case, the last two identities imply

$$|\beta(z)^\gamma-\beta_\tau(z)^\gamma|\le|\beta(z)|^\gamma c\tau|\beta(z)|\le c\tau|z|^{1+\gamma}\quad\text{(here we use (3.8)).}\tag{3.34}$$

If $\tau|\beta(z)|\ge\frac{1}{2}$, then (3.8) and (3.28) imply

$$\tau|z|\ge c\tau|\beta(z)|\ge c\qquad\forall\, z\in\Gamma_{\theta,\kappa}^\tau,\tag{3.35}$$

$$|\beta(z)^\gamma-\beta_\tau(z)^\gamma|\le c|z|^\gamma\le c\tau|z|^{1+\gamma}\qquad\forall\, z\in\Gamma_{\theta,\kappa}^\tau.\tag{3.36}$$

In either case, we have

$$|\beta(z)^\gamma-\beta_\tau(z)^\gamma|\le c\tau|z|^{1+\gamma}\quad\forall\, z\in\Gamma_{\theta,\kappa}^\tau,\tag{3.37}$$

which further implies

$$|\beta(z)^{\alpha-1} - \beta_\tau(z)^{\alpha-1}| \le c\tau|z|^\alpha \qquad \forall\, z \in \Gamma^\tau_{\theta,\kappa}, \tag{3.38}$$

$$|\beta(z)^{1-\alpha} - \beta_\tau(z)^{1-\alpha}| \le c\tau|z|^{2-\alpha} \qquad \forall\, z \in \Gamma^\tau_{\theta,\kappa}, \tag{3.39}$$

$$|\eta(z) - \eta_\tau(z)| = |\beta(z)^\alpha - \beta_\tau(z)^\alpha| \le c\tau|z|^{1+\alpha} \qquad \forall\, z \in \Gamma^\tau_{\theta,\kappa}, \tag{3.40}$$

and

$$\begin{aligned}
&\big\|\big(\eta(z) - \Delta\big)^{-1} - \big(\eta_\tau(z) - \Delta\big)^{-1}\big\|_{M(\Omega)\to M(\Omega)} \\
&= \big\|\big(\eta(z) - \Delta\big)^{-1}\big(\eta(z) - \eta_\tau(z)\big)\big(\eta_\tau(z) - \Delta\big)^{-1}\big\|_{M(\Omega)\to M(\Omega)} \\
&\le c\big\|\big(\eta(z) - \Delta\big)^{-1}\big\|_{M(\Omega)\to M(\Omega)}\|\eta(z) - \eta_\tau(z)\|_{C(\overline{\Omega})}\big\|\big(\eta_\tau(z) - \Delta\big)^{-1}\big\|_{M(\Omega)\to M(\Omega)} \\
&\le c|z|^{-\alpha}\ c\tau|z|^{1+\alpha}\ c|z|^{-\alpha} \quad \text{(use Proposition 3.1(2), Proposition 3.2(2}'\text{), and (3.40))} \\
&\le c\tau|z|^{1-\alpha}.
\end{aligned} \tag{3.41}$$

By using (3.38)-(3.40) and (3.41), we have

$$\begin{aligned}
I_1^* &= \left\|(\beta(z)^{\alpha-1} - \beta_\tau(z)^{\alpha-1})\big(\eta(z) - \Delta\big)^{-1}\left(\beta(z)^{1-\alpha}\frac{G_0\eta(z)}{z - ipU}\right)\right\|_{M(\Omega)} \\
&\le c\tau|z|^\alpha c|z|^{-\alpha}\left(c|z|^{1-\alpha}\frac{c|z|^\alpha}{c|z|}\right)\|G_0\|_{M(\Omega)} \quad \text{(use (3.38), (3.8), and (3.11))} \\
&\le c\|G_0\|_{M(\Omega)}\tau
\end{aligned} \tag{3.42}$$

$$\begin{aligned}
I_2^* &= \left\|\beta_\tau(z)^{\alpha-1}\big((\eta(z) - \Delta)^{-1} - (\eta_\tau(z) - \Delta)^{-1}\big)\left(\beta(z)^{1-\alpha}\frac{G_0\eta(z)}{z - ipU}\right)\right\|_{M(\Omega)} \\
&\le c|z|^{\alpha-1}c\tau|z|^{1-\alpha}\left(c|z|^{1-\alpha}\frac{c|z|^\alpha}{c|z|}\right)\|G_0\|_{M(\Omega)} \quad \text{(use (3.8) and (3.41))} \\
&\le c\|G_0\|_{M(\Omega)}\tau
\end{aligned} \tag{3.43}$$

$$\begin{aligned}
I_3^* &= \left\|\beta_\tau(z)^{\alpha-1}(\eta_\tau(z) - \Delta)^{-1}\left((\beta(z)^{1-\alpha} - \beta_\tau(z)^{1-\alpha})\frac{G_0\eta(z)}{z - ipU}\right)\right\|_{M(\Omega)} \\
&\le c|z|^{\alpha-1}c|z|^{-\alpha}\left(c\tau|z|^{2-\alpha}\frac{c|z|^\alpha}{c|z|}\right)\|G_0\|_{M(\Omega)} \quad \text{(use (3.39), (3.8), and (3.11))} \\
&\le c\|G_0\|_{M(\Omega)}\tau
\end{aligned} \tag{3.44}$$

$$\begin{aligned}
I_4^* &= \left\|\beta_\tau(z)^{\alpha-1}(\eta_\tau(z) - \Delta)^{-1}\left(\beta_\tau(z)^{1-\alpha}\frac{G_0(\eta(z) - \eta_\tau(z))}{z - ipU}\right)\right\|_{M(\Omega)} \\
&\le c|z|^{\alpha-1}c|z|^{-\alpha}\left(c|z|^{1-\alpha}\frac{c\tau|z|^{1+\alpha}}{c|z|}\right)\|G_0\|_{M(\Omega)} \quad \text{(use (3.40), (3.8), and (3.11))} \\
&\le c\|G_0\|_{M(\Omega)}\tau.
\end{aligned} \tag{3.45}$$

Finally, to estimate I_5, we denote $\xi = z - ipU$ and use the Taylor expansions

$$1 - e^{-\tau\xi} = \tau\xi - \tau^2\xi^2 \int_0^1 e^{-\theta\tau\xi}(1-\theta)\mathrm{d}\theta, \tag{3.46}$$

$$\tau\xi e^{-\tau\xi} = \tau\xi - \tau^2\xi^2 \int_0^1 e^{-\theta\tau\xi}\mathrm{d}\theta. \tag{3.47}$$

In the case $\tau|\xi| < \frac{1}{2}$ we have

$$\begin{aligned}\left\|\frac{1}{z-ipU} - \frac{\tau e^{-\tau(z-ipU)}}{1-e^{-\tau(z-ipU)}}\right\| &= \left\|\frac{1}{\xi} - \frac{\tau e^{-\tau\xi}}{1-e^{-\tau\xi}}\right\| \\ &= \left\|\frac{1-e^{-\tau\xi} - \tau\xi e^{-\tau\xi}}{\xi(1-e^{-\tau\xi})}\right\| \\ &= \left\|\frac{\tau^2\xi^2\int_0^1 e^{-\theta\tau\xi}\theta\mathrm{d}\theta}{\tau\xi^2(1-\tau\xi\int_0^1 e^{-\theta\tau\xi}(1-\theta)\mathrm{d}\theta)}\right\| \\ &\le c\tau. \end{aligned} \tag{3.48}$$

In the case $\tau|\xi| \ge \frac{1}{2}$ we have

$$\tau|z| \ge \tau|\xi + ipU(x)| \ge \frac{1}{2} - \tau|p|\|U\|_{C(\overline{\Omega})} \ge \frac{1}{4} \quad \text{when } \tau < \frac{1}{4|p|\|U\|_{C(\overline{\Omega})}},$$

$$c\tau|z| \le |1-e^{-\tau(z-ipU)}| \le c\tau|z| \quad (\text{just as } c|z| \le |\beta_\tau(z)| \le c|z| \text{ proved in (3.28)}),$$

$$\tau|z-ipU| \le c \quad \text{for } z \in \Gamma_{\theta,\kappa}^\tau,$$

which implies

$$\begin{aligned}\left\|\frac{1}{z-ipU} - \frac{\tau e^{-\tau(z-ipU)}}{1-e^{-\tau(z-ipU)}}\right\| &\le \left\|\frac{1}{z-ipU}\right\| + \left\|\frac{\tau e^{-\tau(z-ipU)}}{1-e^{-\tau(z-ipU)}}\right\| \\ &\le \frac{c}{|z|} + \frac{c}{|z|} \\ &\le \frac{c\tau}{\tau|z|} \le c\tau. \end{aligned} \tag{3.49}$$

In either case, we have

$$\left\|\frac{1}{z-ipU} - \frac{\tau e^{-\tau(z-ipU)}}{1-e^{-\tau(z-ipU)}}\right\| \le c\tau. \tag{3.50}$$

Then we have

$$\begin{aligned} I_5^* &= \left\|\beta_\tau(z)^{\alpha-1}(\eta_\tau(z)-\Delta)^{-1}\left(\beta_\tau(z)^{1-\alpha}G_0\eta_\tau(z)\left(\frac{1}{z-ipU} - \frac{\tau e^{-\tau(z-ipU)}}{1-e^{-\tau(z-ipU)}}\right)\right)\right\|_{M(\Omega)} \\ &\le c|z|^{\alpha-1}c|z|^{-\alpha}\big(c|z|^{1-\alpha}c|z|^\alpha c\tau\big)\|G_0\|_{M(\Omega)} \quad (\text{use (3.8), (3.11), and (3.50)}) \\ &\le c\|G_0\|_{M(\Omega)}\tau. \end{aligned} \tag{3.51}$$

Substituting the estimates of I_j^*, $j = 1, \ldots, 5$, into (3.33) yields the result of Lemma 3.4. ∎

Remark 3.3. Let $F(w) = w^{\alpha-1}(w^\alpha - \lambda^\alpha - \Delta)^{-1}w^{1-\alpha}(w^\alpha - \lambda^\alpha)$ and $g(t) = G_0(x)e^{\lambda t}$, which satisfies $\|F(w)\|_{M(\Omega)\to M(\Omega)} \le c$. Intuitively, the following estimate of CQ discretization is a consequence of [19, Theorem 3.1] with $\mu = 0$:

$$\left\| L_w^{-1}[F(w)\widehat{g}] - L_w^{-1}\left[F\left(\frac{1-e^{-\tau w}}{\tau}\right)\widehat{g}\right]\right\|_{M(\Omega)} \le c\|G_0\|_{M(\Omega)} t^{-1}\tau, \tag{3.52}$$

where L_w^{-1} denotes inverse Laplace transform with respect to the variable w. The estimate of J_2 in (3.32) is analogous to (3.52) but not exactly the same. The gap between (3.32) and (3.52) includes

(i) $\widehat{g} = \frac{G_0(x)}{w-\lambda}$ is further approximated by $\widetilde{g} = \frac{G_0(x)\tau e^{-\tau w} e^{\lambda\tau}}{1-e^{-\tau w}e^{\lambda\tau}}$;

(ii) if $U(x)$ =const, then

$$J_2 = e^{(\lambda - ipU)t}\left(L_w^{-1}[F(w)\widehat{g}] - L_w^{-1}\left[F\left(\frac{1-e^{-\tau w}}{\tau}\right)\widetilde{g}\right]\right).$$

However, since $w = z + \lambda - ipU(x)$ is a function of x (instead of a complex constant), it follows that

$$J_2 \ne L_w^{-1}[F(w)\widehat{g}] - L_w^{-1}\left[F\left(\frac{1-e^{-\tau w}}{\tau}\right)\widetilde{g}\right].$$

Therefore we have to prove (3.32) and Lemma 3.4 instead of applying [19, Theorem 3.1] directly;

(iii) [19, Theorem 3.1] was proved for $\mu > 0$.

Remark 3.4. In Theorem 3.3 we have proved the convergence of the numerical solutions under the measure norm. The error estimate presented in this paper can be easily adapted to the case $G_0 \in L^2(\Omega)$ by changing both the norms $\|\cdot\|_{M(\Omega)}$ and $\|\cdot\|_{C(\overline{\Omega})}$ to $\|\cdot\|_{L^2(\Omega)}$ in the proof. In this case we would have the following estimate:

$$\|G(\cdot, t_n) - G_n\|_{L^2(\Omega)} \le c_T \|G_0\|_{L^2(\Omega)}\, t_n^{-1}\tau, \qquad n = 1, 2, \ldots, N. \tag{3.53}$$

4. Technical proofs.

4.1. Proof of Proposition 3.1. In the analysis of (1.1), the analyticity and estimates of the integrands in (2.23) and (2.24) are immediate consequences of the angle property (2.15) and [1, Theorem 3.7.11]. In the analysis of (1.5), however, the analyticity and estimates of the integrands in (3.6) and (3.27) require more technical analysis. In particular, we need to show that

$$\eta(x,z) = (z+\lambda-ipU(x))^\alpha - \lambda^\alpha \in \Sigma_\phi, \quad \eta_\tau(x,z) = \left(\frac{1-e^{-\tau(z+\lambda-ipU(x))}}{\tau}\right)^\alpha - \lambda^\alpha \in \Sigma_\phi$$

for some $\phi \in (\frac{\pi}{2}, \pi)$ in order to apply [1, Theorem 3.7.11]. To this end, we need the following technical lemma, which differs from (2.15) by allowing $|\mathrm{Im}(z)|$ to exceed $\frac{\pi}{\tau}$. The proof of Lemma 4.1 is presented in Appendix A. Roughly speaking, the lemma says that $\arg(\frac{1-e^{-\tau z}}{\tau})$ can be controlled by $|\arg(z)|$ up to $O(\tau)$.

LEMMA 4.1. *Let $L = \lambda + |p|\|U\|_{C(\overline{\Omega})}$. There exist positive constants $\theta_0 \in (\frac{\pi}{2}, \frac{5\pi}{8})$, τ_0, and c_0 such that if $\theta \in (\frac{\pi}{2}, \theta_0)$ and $\tau \in (0, \tau_0]$, then*

(4.1)

$$-|\arg(z)| - c_0\tau \le \arg\left(\frac{1-e^{-\tau z}}{\tau}\right) \le |\arg(z)| + c_0\tau$$

$$\text{if } |z| \ne 0,\ |\arg(z)| \le \theta,\ \text{ and } |\mathrm{Im}(z)| \le \frac{\pi}{\tau} + L\,.$$

Let $\theta \in (\frac{\pi}{2}, \theta_0)$ be a fixed angle. We summarize the results of this section in the following proposition.

Proof of Proposition 3.1(1). For all $z \in \Sigma_{\theta,\kappa}$ and $x \in \Omega$, we have

$$|\arg(\beta(z)) - \arg(z)| = |\arg(z+\lambda - ipU(x)) - \arg(z)| \le \arcsin\bigg(\frac{|\lambda - ipU(x)|}{|z|}\bigg) \le \arcsin\bigg(\frac{|\lambda| + |p|\|U\|_{C(\overline{\Omega})}}{\kappa}\bigg).$$

When κ is large enough compared with $|\lambda| + |p|\|U\|_{C(\overline{\Omega})}$, the angle above is smaller than $\frac{\pi}{8}$ and

$$|z+\lambda - ipU(x)| \ge \kappa - |\lambda - ipU(x)| \ge \frac{3\kappa}{4}.$$

Consequently, we have

$$z+\lambda - ipU(x) \in \Sigma_{\theta+\frac{\pi}{8},\frac{3\kappa}{4}} \quad \text{and} \quad (z+\lambda - ipU(x))^\alpha \in \Sigma_{\alpha(\theta+\frac{\pi}{8}),(\frac{3\kappa}{4})^\alpha} . \tag{4.2}$$

This proves $\beta(z) \in \Sigma_{\frac{3\pi}{4},\frac{\kappa}{2}}$. Similarly, we have

$$\begin{aligned}&|\arg[(z+\lambda - ipU(x))^\alpha - \lambda^\alpha] - \arg[(z+\lambda - ipU(x))^\alpha]| \\ &\quad\le \arcsin\bigg(\frac{\lambda^\alpha}{|z+\lambda - ipU(x)|^\alpha}\bigg) \le \arcsin\bigg(\frac{\lambda^\alpha}{(\frac{3\kappa}{4})^\alpha}\bigg).\end{aligned}$$

When κ is large enough, the angle above is smaller than $\frac{3(1-\alpha)\pi}{4}$ and $(\frac{3\kappa}{4})^\alpha - \lambda^\alpha \ge (\frac{\kappa}{2})^\alpha$. Consequently, we have

$$\eta(z) = (z+\lambda - ipU(x))^\alpha - \lambda^\alpha \in \Sigma_{\alpha(\theta+\frac{\pi}{8})+\frac{3(1-\alpha)\pi}{4},(\frac{\kappa}{2})^\alpha} \subset \Sigma_{\frac{3\pi}{4},\frac{\kappa^\alpha}{2}}. \tag{4.3}$$

(3.8) is a consequence of the fact that $|z|$ dominates λ and $U(x)$ (due to the largeness of κ). ∎

Proof of Proposition 3.1(2). Choose a fixed $x_0 \in \Omega$ and note that Proposition 3.1(1) implies $(z+\lambda - ipU(x_0))^\alpha - \lambda^\alpha \in \Sigma_{\frac{3\pi}{4},\frac{\kappa^\alpha}{2}}$. Hence, the operator

$$\big((z+\lambda - ipU(x_0))^\alpha - \lambda^\alpha - \Delta\big)^{-1} : C(\overline{\Omega}) \to C(\overline{\Omega}) \cap H_0^1(\Omega)$$

is well-defined, satisfying the following basic resolvent estimate:

$$\big\|\big((z+\lambda - ipU(x_0))^\alpha - \lambda^\alpha - \Delta\big)^{-1}\big\|_{C(\overline{\Omega})\to C(\overline{\Omega})} \le c\big|(z+\lambda - ipU(x_0))^\alpha - \lambda^\alpha\big|^{-1}, \tag{4.4}$$

which is a consequence of the analytic semigroup result [30, Theorem 3.3] and the resolvent estimate [1, Theorem 3.7.11]. Since the equation

$$\big((z+\lambda - ipU(x))^\alpha - \lambda^\alpha - \Delta\big)\phi = f \tag{4.5}$$

can be reformulated as

$$\begin{aligned}&\big((z+\lambda - ipU(x_0))^\alpha - \lambda^\alpha - \Delta\big)\phi \\ &\quad= f + \big((z+\lambda - ipU(x_0))^\alpha - (z+\lambda - ipU(x))^\alpha\big)\phi,\end{aligned} \tag{4.6}$$

applying (4.4) to (4.6) yields

$$\begin{aligned}&\big|(z+\lambda - ipU(x_0))^\alpha - \lambda^\alpha\big|\|\phi\|_{C(\overline{\Omega})} \\ &\quad\le c\|f\|_{C(\overline{\Omega})} + c\big|(z+\lambda - ipU(x_0))^\alpha - (z+\lambda - ipU(x))^\alpha\big|\|\phi\|_{C(\overline{\Omega})} \\ &\quad\le c\|f\|_{C(\overline{\Omega})} + c\big|U(x_0) - U(x)\big|^\alpha\|\phi\|_{C(\overline{\Omega})} \le c\|f\|_{C(\overline{\Omega})} + c\|\phi\|_{C(\overline{\Omega})}.\end{aligned}$$

Since $|z| \geq \kappa$ and κ can be chosen to be large compared with λ and $|p| \cdot \|U\|_{C(\overline{\Omega})}$, it follows that

$$\big|(z+\lambda-ipU(x_0))^\alpha-\lambda^\alpha\big| \geq |z|^\alpha - c\lambda^\alpha - c|U(x_0)|^\alpha \geq \frac{1}{2}|z|^\alpha.$$

The last two inequalities imply $\|\phi\|_{C(\overline{\Omega})} \leq c|z|^{-\alpha}\|f\|_{C(\overline{\Omega})} + c|z|^{-\alpha}\|\phi\|_{C(\overline{\Omega})}$. Again, when $|\kappa|$ is larger than some constant, $|z|$ is sufficiently large so that the second term on the right-hand side can be absorbed by the left-hand side. Consequently, we have proved that the solution of (4.5) satisfies $\|\phi\|_{C(\overline{\Omega})} \leq c|z|^{-\alpha}\|f\|_{C(\overline{\Omega})}$. This proves the well-definedness and boundedness of the operator $(\eta(z)-\Delta)^{-1} : C(\overline{\Omega}) \to C(\overline{\Omega})$ for $z \in \Sigma_{\theta,\kappa}$ with

$$\big\|\big(\eta(z)-\Delta\big)^{-1}\big\|_{C(\overline{\Omega})\to C(\overline{\Omega})} \leq c|z|^{-\alpha} \qquad \forall\, z \in \Sigma_{\theta,\kappa}. \tag{4.7}$$

The duality between $M(\Omega)$ and $C(\overline{\Omega})$ immediately implies the extended map $(\eta(z)-\Delta)^{-1} : M(\Omega) \to M(\Omega)$ as well as the resolvent estimate (3.11).

By using (3.11), we have

$$\begin{aligned}
\|\Delta\big(\eta(z)-\Delta\big)^{-1}\|_{M(\Omega)\to M(\Omega)} &= \|-I+\eta(z)\big(\eta(z)-\Delta\big)^{-1}\|_{M(\Omega)\to M(\Omega)}\\
&\leq 1+\|\eta(z)\big(\eta(z)-\Delta\big)^{-1}\|_{M(\Omega)\to M(\Omega)}\\
&\leq 1+c|z|^\alpha\|\big(\eta(z)-\Delta\big)^{-1}\|_{M(\Omega)\to M(\Omega)} \quad \text{(use (3.8) here)}\\
&\leq c \qquad \text{(use (3.11) here).} && (4.8)
\end{aligned}$$

This proves (3.10). The proof of Proposition 3.1(2) is complete. ∎

Proof of Proposition 3.1(3). Note that

$$\begin{aligned}
&\|G(\cdot,t)\|_{M(\Omega)}\\
&\quad\leq c\int_{\Gamma_{\theta,\kappa}} e^{t|z|\cos(\arg(z))}\left\|(\beta(z)^{\alpha-1}\big(\eta(z)-\Delta\big)^{-1}\left(\beta(z)^{1-\alpha}\frac{G_0(x)\eta(z)}{z-ipU(x)}\right)\right\|_{M(\Omega)}|\mathrm{d}z|\\
&\quad\leq c\int_{\Gamma_{\theta,\kappa}} e^{t|z|\cos(\arg(z))}\|\beta(z)^{\alpha-1}\|_{C(\overline{\Omega})}\|\big(\eta(z)-\Delta\big)^{-1}\|_{M(\Omega)\to M(\Omega)}\\
&\qquad\times\left\|\frac{\beta(z)^{1-\alpha}\eta(z)}{z-ipU(x)}\right\|_{C(\overline{\Omega})}\|G_0\|_{M(\Omega)}|\mathrm{d}z|\\
&\quad\leq c\int_{\Gamma_{\theta,\kappa}} e^{t|z|\cos(\arg(z))}c|z|^{\alpha-1}c|z|^{-\alpha}c|\mathrm{d}z|\\
&\qquad\text{(use (3.8) and (3.11); } |z| \text{ dominates } \lambda \text{ and } U(x))\\
&\quad\leq c\int_{\Gamma_{\theta,\kappa}} e^{t|z|\cos(\arg(z))}|z|^{-1}|\mathrm{d}z|\\
&\quad\leq c\int_\kappa^\infty e^{tr\cos(\theta)}r^{-1}\mathrm{d}r + c\int_{-\theta}^{\theta} e^{tr\cos(\varphi)}\kappa^{-1}\kappa\mathrm{d}\varphi\\
&\quad\leq c\int_{\kappa t}^\infty e^{s\cos(\theta)}s^{-1}\mathrm{d}s + c\int_{-\theta}^{\theta} e^{t\kappa\cos(\varphi)}\mathrm{d}\varphi\\
&\quad\leq c+ce^{\kappa T};
\end{aligned}$$

and similarly,

$$
\begin{aligned}
&\|D_tG(\cdot,t)\|_{M(\Omega)}\\
&\quad=\left\|\frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}} e^{tz}\beta(z)^{\alpha}\big(\eta(z)-\Delta\big)^{-1}\left(\beta(z)^{1-\alpha}\frac{G_0(x)\eta(z)}{z-ipU(x)}\right)\mathrm{d}z\right\|_{M(\Omega)}\\
&\quad\le c\int_{\Gamma_{\theta,\kappa}} e^{t|z|\cos(\arg(z))}\left\|(\beta(z)^{\alpha}\big(\eta(z)-\Delta\big)^{-1}\left(\beta(z)^{1-\alpha}\frac{G_0(x)\eta(z)}{z-ipU(x)}\right)\right\|_{M(\Omega)}\mathrm{d}z\\
&\quad\le c\int_{\Gamma_{\theta,\kappa}} e^{t|z|\cos(\arg(z))}\|\beta(z)^{\alpha}\|_{C(\overline{\Omega})}\|\big(\eta(z)-\Delta\big)^{-1}\|_{M(\Omega)\to M(\Omega)}\\
&\qquad\times\left\|\frac{\beta(z)^{1-\alpha}\eta(z)}{z-ipU(x)}\right\|_{C(\overline{\Omega})}\|G_0\|_{M(\Omega)}|\mathrm{d}z|\\
&\quad\le c\int_{\Gamma_{\theta,\kappa}} e^{t|z|\cos(\arg(z))}c|z|^{\alpha}c|z|^{-\alpha}c|\mathrm{d}z|\\
&\qquad\text{(use (3.8) and (3.11); $|z|$ dominates λ and $U(x)$)}\\
&\quad\le c\int_{\Gamma_{\theta,\kappa}} e^{t|z|\cos(\arg(z))}|\mathrm{d}z|\\
&\quad\le c\int_{\kappa}^{\infty} e^{tr\cos(\theta)}\mathrm{d}r+c\int_{-\theta}^{\theta} e^{tr\cos(\varphi)}\kappa\mathrm{d}\varphi\\
&\quad\le ct^{-1}\int_{\kappa t}^{\infty} e^{s\cos(\theta)}\mathrm{d}s+c\int_{-\theta}^{\theta} e^{t\kappa\cos(\varphi)}\kappa\mathrm{d}\varphi\\
&\quad\le ct^{-1}+c\kappa e^{\kappa T}.
\end{aligned}
$$

Similarly, we also have

$$
\begin{aligned}
&\|\Delta D_t^{1-\alpha}G(\cdot,t)\|_{M(\Omega)}\\
&\quad=\left\|\frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}} e^{tz}\Delta\big(\eta(z)-\Delta\big)^{-1}\left(\beta(z)^{1-\alpha}\frac{G_0(x)\eta(z)}{z-ipU(x)}\right)\right\|_{M(\Omega)}\mathrm{d}z\\
&\quad\le c\int_{\Gamma_{\theta,\kappa}} e^{t|z|\cos(\arg(z))}\left\|\Delta\big(\eta(z)-\Delta\big)^{-1}\left(\beta(z)^{1-\alpha}\frac{G_0(x)\eta(z)}{z-ipU(x)}\right)\right\|_{M(\Omega)}\mathrm{d}z\\
&\quad\le c\int_{\Gamma_{\theta,\kappa}} e^{t|z|\cos(\arg(z))}\|\Delta\big(\eta(z)-\Delta\big)^{-1}\|_{M(\Omega)\to M(\Omega)}\\
&\qquad\times\left\|\beta(z)^{1-\alpha}\frac{\eta(z)}{z-ipU(x)}\right\|_{C(\overline{\Omega})}\|G_0\|_{M(\Omega)}|\mathrm{d}z|\\
&\quad\le c\int_{\Gamma_{\theta,\kappa}} e^{t|z|\cos(\arg(z))}c\|G_0\|_{M(\Omega)}|\mathrm{d}z|\qquad\text{(here we used (3.10) and (3.8))}\\
&\quad\le c\int_{\kappa}^{\infty} e^{tr\cos(\theta)}\mathrm{d}r+c\int_{-\theta}^{\theta} e^{t\kappa\cos(\varphi)}\kappa\mathrm{d}\varphi\\
&\quad\le ct^{-1}\int_{\kappa t}^{\infty} e^{s\cos(\theta)}s^{-\alpha}\mathrm{d}s+c\int_{-\theta}^{\theta} e^{t\kappa\cos(\varphi)}\kappa\mathrm{d}\varphi\\
&\quad\le c(t^{-1}+\kappa e^{\kappa T}).
\end{aligned}
$$

In the same way, one also can prove $\|D_t^{1-\alpha}G(\cdot,t)\|_{M(\Omega)}\le c(t^{\alpha-1}+\kappa e^{\kappa T})$.

Applying the differential operators to the integral representation (3.7) yields that the solution $G(x,t)$ satisfies (1.5) with each term well-defined in $M(\Omega)$. ∎

4.2. Proof of Proposition 3.2. We start with proving (3.28). Let $w = z + \lambda - ipU(x)$, with $z \in \Sigma_{\theta,\kappa}^{\tau}$. For sufficiently small step size $\tau < \frac{\pi}{2\lambda + 2|p|\|U\|_{C(\overline{\Omega})}}$, we have

$$\tau|\mathrm{Im}(w)| < \tau(|\mathrm{Im}(z)| + \lambda + |p|\|U\|_{C(\overline{\Omega})}) \leq \pi + \tau(\lambda + |p|\|U\|_{C(\overline{\Omega})}) < \frac{3}{2}\pi. \tag{4.9}$$

Hence, $1 - e^{-\tau w} = 0$ only when $\omega = 0$. In particular,

$$\text{if } \tau|w| \geq c, \text{ then } |1 - e^{-\tau w}| \geq c. \tag{4.10}$$

For $z \in \Sigma_{\theta,\kappa}^{\tau}$, we have $\tau|\mathrm{Im}(z)| \leq \pi$ and $\tau|\mathrm{Re}(z)| \leq \tau(\kappa + 1) \leq \pi$ when $\tau \leq \frac{\pi}{\kappa+1}$. Consequently, we have

$$\tau|z| \leq \tau|\mathrm{Im}(z)| + \tau|\mathrm{Re}(z)| \leq 2\pi, \tag{4.11}$$

$$\tau|w| \leq \tau|z| + \tau(\lambda + |p|\|U\|_{C(\overline{\Omega})}) \leq \frac{5}{2}\pi. \tag{4.12}$$

By choosing $\kappa \geq 2(\lambda + |p|\|U\|_{C(\overline{\Omega})})$, Taylor's expansion yields, for $z \in \Sigma_{\theta,\kappa}^{\tau}$,

$$|\beta_\tau(z)| = \left|\frac{1 - e^{-\tau w}}{\tau}\right| \leq c|w| \leq c(|z| + \lambda + |p|\|U\|_{C(\overline{\Omega})}) \leq c(|z| + \kappa) \leq c|z|, \tag{4.13}$$

where the last inequality is a consequence of $|z| \geq \kappa$ for $z \in \Sigma_{\theta,\kappa}^{\tau}$. This proves the inequality $|\beta_\tau(z)| \leq c|z|$ in (3.28).

To prove $c|z| \leq |\beta_\tau(z)|$ for $z \in \Sigma_{\theta,\kappa}^{\tau}$, we consider two cases below.

If $\tau|w|$ is smaller than some constant, then we can use Taylor's expansion (with $|O(\tau w)| < \frac{1}{2}$, due to the smallness of $\tau|w|$ assumed):

$$\begin{aligned} |\beta_\tau(z)| = \left|\frac{1 - e^{-\tau w}}{\tau}\right| = |w(1 + O(\tau w))| \geq \frac{1}{2}|w| &\geq \frac{1}{2}(|z| - \lambda - |p|\|U\|_{C(\overline{\Omega})}) \\ &\geq \frac{1}{2}(|z| - \kappa/2) \geq \frac{1}{4}|z|, \end{aligned} \tag{4.14}$$

where we have used $\kappa \geq 2(\lambda + |p|\|U\|_{C(\overline{\Omega})})$ again and noted that $|z| \geq \kappa$ for $z \in \Sigma_{\theta,\kappa}^{\tau}$.

If $\tau|w|$ is larger than the constant, then (4.10) and (4.11) imply

$$|\beta_\tau(z)| = \left|\frac{1 - e^{-\tau w}}{\tau}\right| \geq \frac{c}{\tau} \geq c|z|. \tag{4.15}$$

Overall, under the conditions $\kappa \geq 2(\lambda + |p|\|U\|_{C(\overline{\Omega})})$ and $\tau < \frac{\pi}{\kappa+1}$, we have proved

$$c_1|z| \leq |\beta_\tau(z)| = \left|\frac{1 - e^{-\tau(z+\lambda-ipU(x))}}{\tau}\right| \leq c_2|z| \quad \forall\, z \in \Sigma_{\theta,\kappa}^{\tau} \tag{4.16}$$

for some positive constants c_1 and c_2. The last inequality further implies

$$c_1|z|^\alpha - \lambda^\alpha \leq \left|\left(\frac{1 - e^{-\tau(z+\lambda-ipU(x))}}{\tau}\right)^\alpha - \lambda^\alpha\right| \leq c_2|z|^\alpha + \lambda^\alpha. \tag{4.17}$$

By choosing κ larger than some constant (depending on λ and $|p|\|U\|_{C(\overline{\Omega})}$), we have $\lambda^\alpha \leq \frac{c_1}{2}\kappa^\alpha \leq \frac{c_1}{2}|z|^\alpha$. Consequently, (4.17) implies

$$\frac{c_1}{2}|z|^\alpha \leq |\eta_\tau(z)| = \left|\left(\frac{1 - e^{-\tau(z+\lambda-ipU(x))}}{\tau}\right)^\alpha - \lambda^\alpha\right| \leq \left(\frac{c_1}{2} + c_2\right)|z|^\alpha. \tag{4.18}$$

The proof of (3.28) is complete. Next, we prove $\beta_\tau(z), \eta_\tau(z) \in \Sigma_{\frac{3\pi}{4}}$ for $z \in \Sigma^\tau_{\theta,\kappa}$. Lemma 4.1 implies

$$
\begin{aligned}
-|\arg(z+\lambda - ipU(x)| - c_0\tau &\le \arg\left(\frac{1-e^{-\tau(z+\lambda-ipU(x))}}{\tau}\right) \\
&\le |\arg(z+\lambda-ipU(x))| + c_0\tau,
\end{aligned} \tag{4.19}
$$

which together with (4.2) implies $-\frac{5\pi}{8} - c_0\tau \le \arg\left(\frac{1-e^{-\tau(z+\lambda-ipU(x))}}{\tau}\right) \le \frac{5\pi}{8} + c_0\tau$. This proves $\beta_\tau(z) \in \Sigma_{\frac{3\pi}{4}}$ when the step size τ is smaller than some constant. Furthermore, by choosing κ large enough and using (4.16) we have

$$
\left|\frac{1-e^{-\tau(z+\lambda-ipU(x))}}{\tau}\right| = |\beta_\tau(z)| \ge c|z| \ge c\kappa \quad \forall\, z \in \Sigma^\tau_{\theta,\kappa}. \tag{4.20}
$$

The last two inequalities yield

$$
\frac{1-e^{-\tau(z+\lambda-ipU(x))}}{\tau} \in \Sigma_{\frac{3\pi}{4},c\kappa} \quad \text{and} \quad \left(\frac{1-e^{-\tau(z+\lambda-ipU(x))}}{\tau}\right)^\alpha \in \Sigma_{\frac{3\alpha\pi}{4},c^\alpha\kappa^\alpha}, \tag{4.21}
$$

which further implies that (by choosing κ to be large enough and using the same argument for (4.3))

$$
\eta_\tau(z) = \left(\frac{1-e^{-\tau(z+\lambda-ipU(x))}}{\tau}\right)^\alpha - \lambda^\alpha \in \Sigma_{\frac{3\pi}{4},c\kappa^\alpha} \subset \Sigma_{\frac{3\pi}{4}}\ . \tag{4.22}
$$

This completes the proof of Proposition 3.2(1′). Using the results $\beta_\tau(z), \eta_\tau(z) \in \Sigma_{\frac{3\pi}{4}}$, Proposition 3.2(2′) can be proved in the same way as (2) of Proposition 3.1. The details are omitted. ∎

5. Numerical tests. In this section, we test the convergence of the time discretization method (3.23) numerically. We solve (1.5) in the one-dimensional domain $\Omega = (0, 1)$ by the proposed method up to time $T = 1$, with the following parameters:

$$
\lambda = 0.01, \quad p = 1, \quad U(x) = x, \tag{5.1}
$$

where the choice of the function $U(x) = x$ physically corresponds to the distribution of the time average of the particles' trajectories. The numerical results with smooth initial data $G(x, 0) = 10x(1-x)$ and measure data $G(x, 0) = \delta(x-1/4)$ are presented in Tables 1 and 2, respectively, where G^N_τ denotes the numerical solution with step size τ at time $t_N = 1$. Since the exact solutions of these problems are unknown, the order of convergence of the numerical solutions are computed by the formula

$$
\text{order of convergence in the norm } \|\cdot\| = \frac{\ln\left(\|G^N_{2\tau} - G^N_\tau\| / \|G^N_\tau - G^N_{\tau/2}\|\right)}{\ln 2}.
$$

To investigate the convergence in time and eliminate the influence from spatial discretization, we use the P1 finite element method with a sufficiently small mesh size $h = 1/500$ so that the error due to spatial discretization can be omitted (roughly 10^{-6} based on numerical tests). Since the two norms $\|\cdot\|_{M(\Omega)}$ and $\|\cdot\|_{L^1(\Omega)}$ are the same for finite element solutions, the norm $\|G^N_\tau - G^N_{\tau/2}\|_{M(\Omega)}$ can be calculated via integration (with 5-node Gauss quadrature on each subinterval, which yields sufficiently accurate results). From Tables 1–2 we see that the proposed method has first-order convergence, which is consistent with the theoretical analysis presented in Theorem 3.3.

Table 1
Order of convergence when the initial data are smooth: $G(x,0) = 10x(1-x)$.

	τ	$\|G_\tau^N - G_{\tau/2}^N\|_{L^2(\Omega)}$	$\frac{\|G_{2\tau}^N - G_\tau^N\|_{L^2(\Omega)}}{\|G_\tau^N - G_{\tau/2}^N\|_{L^2(\Omega)}}$	Order
$\alpha = 0.25$	1/8	1.609E-03	—	—
	1/16	7.913E-04	2.034	1.02
	1/32	3.923E-04	2.016	1.01
	1/64	1.953E-04	2.008	1.00
$\alpha = 0.5$	1/8	2.733E-03	—	—
	1/16	1.310E-03	2.085	1.06
	1/32	6.419E-04	2.041	1.03
	1/64	3.177E-04	2.020	1.01
$\alpha = 0.75$	1/8	3.381E-03	—	—
	1/16	1.535E-03	2.202	1.14
	1/32	7.328E-04	2.095	1.07
	1/64	3.582E-04	2.046	1.03

Table 2
Order of convergence when the initial data are a measure: $G(x,0) = \delta(x-1/4)$.

	τ	$\|G_\tau^N - G_{\tau/2}^N\|_{M(\Omega)}$	$\frac{\|G_{2\tau}^N - G_\tau^N\|_{M(\Omega)}}{\|G_\tau^N - G_{\tau/2}^N\|_{M(\Omega)}}$	Order
$\alpha = 0.25$	1/8	1.058E-03	—	—
	1/16	5.194E-04	2.037	1.03
	1/32	2.574E-04	2.018	1.01
	1/64	1.281E-04	2.009	1.01
$\alpha = 0.5$	1/8	1.553E-03	—	—
	1/16	7.452E-04	2.083	1.06
	1/32	3.653E-04	2.040	1.03
	1/64	1.808E-04	2.020	1.01
$\alpha = 0.75$	1/8	1.772E-03	—	—
	1/16	8.061E-04	2.198	1.14
	1/32	3.852E-04	2.093	1.06
	1/64	1.884E-04	2.045	1.03

6. Conclusion. In this article, we have developed time discretization method for approximating the mild solution of the tempered fractional Feynman–Kac equation based on convolution quadrature approximation of the fractional substantial derivative. We have proved first-order convergence of the numerical method with $U \in C(\overline{\Omega})$ and the initial data G_0 being a finite measure.

If $U(x)$ is second-order continuously differentiable, then by letting $u(x,t) = e^{t(\lambda - ipU(x))}G(x,t)$ and using (3.13), the tempered fractional Feynman–Kac equation can be rewritten as

$$\partial_t u - \Delta \partial_t^{1-\alpha} u - \frac{2}{f}\nabla f \cdot \partial_t^{1-\alpha}\nabla u - \left(\lambda^\alpha + \frac{\Delta f}{f}\right)\partial_t^{1-\alpha} u = F \tag{6.1}$$

with

(6.2)
$$f(x,t) = e^{-t(\lambda - ipU(x))} \quad \text{and} \quad F(x,t) = -G_0(x)(\lambda^\alpha \partial_t^{1-\alpha} - \lambda)e^{\lambda t} = O(t^{\alpha-1}) \quad \text{as} \quad t \to 0.$$

It is worth mentioning that a uniform-in-time $O(\tau^\alpha)$ convergence of a time discretization method for (6.1) can be proved analogously to [16, Theorem 4.4] in the case $\alpha \in (\frac{1}{2}, 1]$.

Appendix A. Proof of Lemma 4.1. It is clear that if $|z| \neq 0$ and $\arg(z) = 0$, then $\arg(\frac{1-e^{-\tau z}}{\tau}) = 0$.

If $|z| \neq 0$ and $\arg(z) = \varphi \in (0, \theta]$ and $0 \le \mathrm{Im}(z) \le \pi/\tau + L$, then $\omega := \tau|z|\sin(\varphi) \in (0, \pi + L\tau]$ and it is easy to see that

Case 1: if $\omega \in (0, \pi]$, then $\arg(\frac{1-e^{-\tau z}}{\tau}) \in [0, \pi)$;

Case 2: if $\omega \in (\pi, \pi + L\tau]$, then $\exists$ a constant c_0 such that $\arg(\frac{1-e^{-\tau z}}{\tau}) \in [-c_0\tau, 0)$.

In Case 2, (4.1) holds automatically.

In Case 1, if $\omega = \pi$, then $\arg(\frac{1-e^{-\tau z}}{\tau}) = 0$ and (4.1) holds. If $\omega \in (0, \pi)$, then we have $\arg(\frac{1-e^{-\tau z}}{\tau}) \in (0, \pi)$ and we prove $\arg(\frac{1-e^{-\tau z}}{\tau}) \le \varphi$ below (then (4.1) follows immediately).

Note that

$$\begin{aligned}\cot\left(\arg\left(\frac{1-e^{-\tau z}}{\tau}\right)\right) &= \frac{1 - e^{-\tau|z|\cos(\varphi)}\cos(\tau|z|\sin(\varphi))}{e^{-\tau|z|\cos(\varphi)}\sin(\tau|z|\sin(\varphi))} \\ &= \frac{e^{\tau|z|\cos(\varphi)} - \cos(\tau|z|\sin(\varphi))}{\sin(\tau|z|\sin(\varphi))} \\ &\ge \frac{1 + \tau|z|\cos(\varphi) - \cos(\tau|z|\sin(\varphi))}{\sin(\tau|z|\sin(\varphi))} = \frac{1 + \omega\cot(\varphi) - \cos(\omega)}{\sin(\omega)},\end{aligned}$$

where we have used Taylor's expansion in the last inequality and set $\omega = \tau|z|\sin(\varphi) \in (0, \pi)$. We shall prove $\cot(\arg(\frac{1-e^{-\tau z}}{\tau})) \ge \cot(\varphi)$ for $\omega \in (0, \pi)$, so that $0 \le \arg(\frac{1-e^{-\tau z}}{\tau}) \le \varphi = \arg(z)$. To this end, we consider the function

$$f(\omega) := 1 + \omega\cot(\varphi) - \cos(\omega) - \sin(\omega)\cot(\varphi), \quad \omega \in [0, \pi]$$

with fixed φ and variable ω (due to the change of $|z|$). The derivative of f is

$$\begin{aligned}f'(\omega) &= \sin(\omega) + (1 - \cos(\omega))\cot(\varphi) \\ &= 2\sin\left(\frac{\omega}{2}\right)\cos\left(\frac{\omega}{2}\right) + 2\sin^2\left(\frac{\omega}{2}\right)\cot(\varphi) = 2\sin^2\left(\frac{\omega}{2}\right)\left(\cot\left(\frac{\omega}{2}\right) + \cot(\varphi)\right).\end{aligned}$$

If $\varphi \in (0, \frac{\pi}{2}]$, then $f'(\omega) > 0$ for $\omega \in (0, \pi)$, which means that the minimum value of f is achieved at $f(0) = 0$. If $\varphi \in (\frac{\pi}{2}, \theta]$, then $f'(\omega) > 0$ for $\omega \in (0, \pi - \varphi)$ and $f'(\omega) < 0$ for $\omega \in (\pi - \varphi, \pi]$, which means that the minimum value of f is achieved at either $f(0) = 0$ or $f(\pi) = 2 + \omega\cot(\varphi)$. In either case, the minimum value of f is achieved at one of the two end points, $\omega = 0$ and $\omega = \pi$ with

$$f(0) = 0 \quad \text{and} \quad f(\pi) = 2 + \pi\cot(\varphi).$$

By choosing $\theta \in (\frac{\pi}{2}, \pi)$ sufficiently close to $\frac{\pi}{2}$ we have $f(\pi) \ge 0$. Consequently, $f(\omega) \ge 0$ for all $\omega \in (0, \pi)$. This proves $\cot(\arg(\frac{1-e^{-\tau z}}{\tau})) \ge \cot(\varphi)$ for all $\omega \in (0, \pi)$, which yields $\arg(\frac{1-e^{-\tau z}}{\tau}) \le \varphi$, completing the proof of Case 1.

Overall, we have proved (4.1) in the case $\arg(z) \in [0, \theta]$. The case $\arg(z) \in [-\theta, 0)$ can be proved in the same way.

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