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REGULARITY THEORY AND NUMERICAL ALGORITHM FOR THE TIME-FRACTIONAL KLEIN-KRAMERS EQUATION*

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Abstract

Fractional Klein-Kramers equation can well describe subdiffusion in phase space. In this paper, we develop the fully discrete scheme for time-fractional Klein-Kramers equation based on the backward Euler convolution quadrature and local discontinuous Galerkin methods. Thanks to the obtained sharp regularity estimates in temporal and spatial directions after overcoming the hypocoercivity of the operator, the complete error analyses of the fully discrete scheme are built. It is worth mentioning that the convergence of the provided scheme is independent of the temporal regularity of the exact solution. Finally, numerical results are proposed to verify the correctness of the theoretical results.

Mathematics subject classification: 65M60, 35R11, 65M12, 65M15.
Key words: Time-fractional Klein-Kramers equation, Regularity estimate, Convolution quadrature, Local discontinuous Galerkin method, Error analysis.

1. Introduction

Subdiffusion is ubiquitous in the nature world [18]. Microscopically, it can be modeled by Langevin dynamics with long-tailed trapping [19]. To describe how the presence of the trapping events leads to the macroscopic observation of subdiffusion, the authors establish the fractional Klein-Kramers equation [17, 19]. This paper is concerned with the regularity estimate and numerical analysis for the time-fractional Klein-Kramers equation, i.e.

$$\partial_t G(x,v,t) + {}_0\partial_t^{1-\alpha}\left(\gamma v\frac{\partial}{\partial x} - \gamma\frac{\partial}{\partial v}\eta v - \frac{\gamma\eta}{m\beta}\frac{\partial^2}{\partial v^2}\right)G(x,v,t) = {}_0\partial_t^{1-\alpha} f, \qquad \big((x,v),t\big)\in\Omega\times(0,T] \tag{1.1}$$

with the initial condition

$$G(x,v,0) = G_0, \quad (x,v)\in\Omega,$$

and the boundary conditions

$$\begin{aligned} &G(x,0,t) = G(x,1,t) = 0, && (x,t)\in(0,1)\times(0,T],\\ &G(0,v,t) = 0, && (v,t)\in(0,1)\times(0,T]. \end{aligned} \tag{1.2}$$

Here $\Omega = \{(x,v)\,|\,0<x<1,\ 0<v<1\}$, T denotes the fixed terminal time, f is source term, v is the velocity, η is the friction constant, m is the mass of the particle, γ is the ratio of the

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intertrapping time scale and the internal waiting time scale, and β is a variable related to the temperature and Boltzmann's constant, without loss of generality, we take $\eta = \beta = m = \gamma = 1$ in the following, ${}_0\partial_t^{1-\alpha}$ is the Riemann-Liouville fractional derivative with $\alpha \in (0,1)$ defined by [21]

$$
{}_0\partial_t^{1-\alpha} G = \frac{1}{\Gamma(\alpha)} \frac{\partial}{\partial t} \int_0^t (t-\xi)^{\alpha-1} G(\xi) d\xi. \tag{1.3}
$$

In the past few years, there have been some discussions for solving fractional Klein-Kramers equation numerically [6, 10, 13, 20]. In [6], the authors consider the finite difference scheme for the time-fractional Klein-Kramers equation and provide the corresponding error analyses. Reference [20] provides a hybrid algorithm using the local radial basis functions based on finite difference to obtain the numerical solution of the time-fractional Klein-Kramers equation; the authors use finite difference scheme to solve space-fractional Klein-Kramers equation with Riesz fractional derivative in [13]. From the above works, it can be noted that the corresponding numerical discussions in Galerkin framework for fractional Klein-Kramers equation are rare.

In this paper, we first build the regularity of the Eq. (1.1), and then present the robust numerical scheme and complete error analyses. As for the regularity estimates, to overcome the challenges caused by the hypocoercivity of the operator $(v(\partial/\partial x) - (\partial/\partial v)v - \partial^2/\partial v^2)$, we introduce a new operator $\mathcal{L}$ (one can refer to (2.1)) and provide the corresponding resolvent estimate (see Lemma 2.1); with the help of equivalent form of (1.1) and resolvent estimate, we find

$$
\begin{aligned}
&\|G(t)\|_{L^2(\Omega)} \le C\|G_0\|_{L^2(\Omega)} + C\|f(0)\|_{L^2(\Omega)} + C\int_0^t \|f'(s)\|_{L^2(\Omega)} ds, \\
&\|G'(t)\|_{L^2(\Omega)} \le Ct^{-1}\|G_0\|_{L^2(\Omega)} + Ct^{\alpha-1}\|f(0)\|_{L^2(\Omega)} + C\int_0^t (t-s)^{\alpha-1}\|f'(s)\|_{L^2(\Omega)} ds.
\end{aligned}
$$

Next we use backward Euler convolution quadrature to discretize the temporal derivative and an $\mathcal{O}(\tau)$ convergence rate is obtained without any regularity assumptions on the exact solution. At last, we use local discontinuous Galerkin method to discretize spatial derivative; to obtain the stability and the convergence of the fully-discrete scheme, we build a new discrete Grönwall's inequality (see Lemma 4.1 for the details).

The plan of the paper is as follows. Next, we provide the regularity of the time-fractional Klein-Kramers equation in temporal and spatial directions, respectively. In Section 3, the time semi-discrete scheme is built by backward Euler convolution quadrature and the resulting error analysis is also provided. Then we use the local discontinuous Galerkin method to discretize the space operator and the error estimate is obtained in Section 4. Section 5 validates the effectiveness of the algorithm by extensive numerical experiments. We conclude the paper with some discussions in the last section. Throughout the paper, C is a positive constant, whose value may differ at different places, $\|\cdot\|$ stands for the operator norm from $L^2(\Omega)$ to $L^2(\Omega)$, and "~" means Laplace transform.

2. Regularity of the Solution

Here we first provide some notations, and then present the solution and discuss its regularity. Define $\Gamma_{\theta,\kappa}$ for $\kappa > 0$ and $\theta \in (\pi/2, \pi)$ as

$$
\Gamma_{\theta,\kappa} = \left\{ re^{-\mathbf{i}\theta} : r \ge \kappa \right\} \cup \left\{ \kappa e^{\mathbf{i}\omega} : |\omega| \le \theta \right\} \cup \left\{ re^{\mathbf{i}\theta} : r \ge \kappa \right\},
$$