

# 分数阶 Cahn-Hilliard 方程的高效数值算法<sup>\*</sup>

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**摘要:** 给出了时空分数阶 Cahn-Hilliard 方程的一个高效数值算法. 首先, 利用 Laplace 变换将时空分数阶 Cahn-Hilliard 方程转化为空间分数阶 Cahn-Hilliard 方程; 然后, 结合 Fourier 谱方法和有限差分法得到一个时间二阶、空间谱精度的高效数值格式; 最后, 通过数值实验验证本文数值算法的有效性, 并验证其满足能量耗散性质和质量守恒定律.

**关键词:** 分数阶 Cahn-Hilliard 方程; Laplace 变换; Fourier 谱方法; 有限差分法; 能量耗散; 质量守恒

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## An Efficient Numerical Algorithm for Fractional Cahn-Hilliard Equations

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**Abstract:** An efficient numerical algorithm for the time-space fractional Cahn-Hilliard equation was proposed. Firstly, the time-space fractional Cahn-Hilliard equation was converted into the spatial fractional Cahn-Hilliard equation through the Laplace transform. Then, by means of the Fourier spectral method combined with the finite difference method, an efficient numerical scheme with 2nd-order convergence in time and spectral accuracy in space was obtained. Finally, the validity of the proposed algorithm was verified by numerical experiments. The algorithm satisfies the energy dissipation law and the mass conservation law.

**Key words:** fractional Cahn-Hilliard equation; Laplace transform; Fourier spectral method; finite difference method; energy dissipation; mass conservation

## 引言

1958 年, Cahn 和 Hilliard<sup>[1-2]</sup> 引入 Cahn-Hilliard (CH) 方程, 用来描述固体中复杂的相分离和粗化现象, 该

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方程还在材料科学<sup>[3]</sup>、图像处理<sup>[4]</sup>等领域有着广泛的应用. CH 方程是刚性的、四阶的、非线性的,并且具有多个时间尺度和空间尺度,很难准确求解.因此,研究这一问题的有效数值计算方法具有其现实意义,同时也引起了许多研究者的关注,且取得了许多研究成果,如有限差分法<sup>[5-6]</sup>、有限元方法<sup>[7]</sup>、有限体积法<sup>[8]</sup>及谱方法<sup>[9-10]</sup>等.

近年来,分数阶微分方程的数值算法研究也引起了学者们的关注<sup>[11-12]</sup>.分数阶微分算子的概念由来已久,最早出现在 1695 年德国数学家 Leibniz 写给法国数学家 l'Hôpital 的信中.分数阶模型也是非局部模型,它具有的历史依赖和非局部的特性使其可以比整数阶方程更有效地描述一些复杂系统<sup>[13-15]</sup>.分数阶模型为描述复杂现象提供了新的角度,它也成为研究这些复杂系统的重要工具.分数阶微分方程是传统微分方程的推广,且通常被用作与超扩散(空间分数阶)、亚扩散(时间分数阶)或与两者有关<sup>[16]</sup>的扩散过程的建模工具.分数阶微分方程在地下水资源<sup>[17]</sup>、运输动力学<sup>[18]</sup>、金融学<sup>[19]</sup>、混沌理论<sup>[20]</sup>和磁性资源<sup>[21]</sup>等领域研究中也有着广泛应用.本文考虑如下形式的时空分数阶 CH 方程:

$$\begin{cases} \frac{\partial^\alpha u}{\partial t^\alpha} = \Delta(\varepsilon(-\Delta)^{\beta/2}u + f(u)), & (x, t) \in \Omega \times (0, T], \\ u(x, 0) = u_0, & x \in \Omega, \end{cases} \quad (1)$$

其中,  $\partial^\alpha u / \partial t^\alpha$  为 Caputo 型分数阶导数,  $(-\Delta)^{\beta/2}$  为分数阶 Laplace 算子,且  $\alpha \in (0, 1]$ ,  $\beta \in (1, 2]$ , 非线性项  $f(u) = u^3 - u$ , 边界条件取周期边界条件.分数阶 CH 方程还可视为分数阶意义下 Ginzburg-Landau 能量泛函的  $H^{-1}$  梯度流<sup>[22]</sup>, 即

$$E^\beta(u) = \int_\Omega \left( \frac{\varepsilon}{2} u(-\Delta)^{\beta/2}u + F(u) \right) dx, \quad (2)$$

其中,  $F(u) = (u^2 - 1)^2/4$ , 且分数阶 CH 方程(1)满足能量耗散性质<sup>[23-24]</sup>.

除此之外,与整数阶 CH 方程类似,分数阶 CH 方程满足质量守恒律,即

$$M(u(t)) = M(u_0). \quad (3)$$

同样,关于分数阶 CH 方程的数值算法,目前也已经取得了许多研究成果.Weng 等<sup>[25]</sup>通过引入稳定化项,给出了空间分数阶 CH 方程的一个基于 Fourier 谱的无条件能量稳定的非线性数值格式;Zhai 等<sup>[26]</sup>利用算子分裂法得到了一个求解分数阶 CH 方程的高效数值格式;Bosch 和 Stoll<sup>[27]</sup>将分数阶 CH 模型用于二值图像的绘制,并针对该模型给出了一种基于 Fourier 谱方法的一阶凸分裂隐格式;Zhang 等<sup>[28]</sup>给出了求解时间分数阶 CH 方程的一个非一致时间步长下的凸分裂格式;Ainsworth 和 Mao<sup>[22]</sup>还给出了分数阶 CH 方程的稳定性分析.

本文基于 Fourier 谱方法和有限差分法,给出了一个求解时空分数阶 CH 方程的一个高效数值算法.首先,利用 Laplace 变换将时空分数阶 CH 方程转化为空间分数阶 CH 方程;再结合 Fourier 谱方法及有限差分法(Crank-Nicolson 格式),得到了一个精度较高的数值格式;最后,通过数值算例验证了数值格式的高效性,并验证其满足能量耗散性质及质量守恒.

## 1 分数阶 CH 方程的高效数值算法

### 1.1 Laplace 变换

函数  $f(t)$  的 Laplace 变换的定义表达式为<sup>[29]</sup>

$$F(s) = L\{f(t); s\} = \int_0^\infty e^{-st} f(t) dt,$$

且有如下的原函数微分性质:

$$L[f^{(k)}(t)] = s^k L[f(t)] - s^{k-1}f(0) - s^{k-2}f'(0) - \dots - f^{(k-1)}(0). \quad (4)$$

类似地, Caputo 型分数阶导数的 Laplace 变换为<sup>[29]</sup>

$$L[{}_0^C D_t^p f(t)] = s^p F(s) - \sum_{k=0}^{n-1} s^{p-k-1} f^{(k)}(0), \quad n-1 < p \leq n, \quad (5)$$

且当  $n = 1$  时,即  $0 < p \leq 1$  时,有

$$L[{}_0^C D_t^\rho f(t)] = s^\rho F(s) - s^{\rho-1} f(0).$$

对  $s^\rho$  做线性插值, 再结合 Laplace 逆变换<sup>[30]</sup> 得

$${}_0^C D_t^\rho f(t) \approx pf'(t) + (1-p)[f(t) - f(0)]. \quad (6)$$

从而, CH 方程(1)中的 Caputo 型时间分数阶导数可做如下近似:

$$\frac{\partial^\alpha u}{\partial t^\alpha} \approx \alpha \frac{\partial u(x,t)}{\partial t} + (1-\alpha)[u(x,t) - u(x,0)]. \quad (7)$$

最终可将时空分数阶问题转化为如下空间分数阶问题:

$$\alpha u_t + (1-\alpha)(u - u_0) = \Delta(\varepsilon(-\Delta)^{\beta/2} u + f(u)),$$

整理得

$$u_t = \frac{\alpha-1}{\alpha}(u - u_0) + \frac{1}{\alpha}\Delta(\varepsilon(-\Delta)^{\beta/2} u + f(u)). \quad (8)$$

## 1.2 空间逼近: Fourier 谱方法

考虑空间区域  $\Omega = [a, b] \times [a, b]$ , 并做如下的网格剖分:

$$\Omega_h^{\text{per}} = \{(x_i, y_j) = (a + ih, a + jh), 0 \leq i, j \leq M-1\},$$

其中  $h = (b-a)/M$ .

谱分解对分数阶 Laplace 算子的离散有着十分重要的作用<sup>[31-32]</sup>. 假设对二维 Laplace 算子  $(-\Delta)$ , 存在一组标准正交特征函数  $\varphi_{pq}$ , 且满足有界区域  $[a, b]^2$  上的标准边界条件, 记相应特征值为  $\lambda_{pq}$ , 则  $(-\Delta)\varphi_{pq} = \lambda_{pq}\varphi_{pq}$ . 令

$$U_\beta = \left\{ u = \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} \hat{u}_{pq} \varphi_{pq}, \hat{u}_{pq} = \langle u, \varphi_{pq} \rangle, \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} |\hat{u}_{pq}|^2 |\lambda_{pq}|^{\beta/2} < \infty, 1 < \beta \leq 2 \right\}. \quad (9)$$

而分数阶 Laplace 算子  $(-\Delta)^{\beta/2}$  也有类似的谱分解<sup>[16]</sup>, 即

$$(-\Delta)^{\beta/2} u = \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} \hat{u}_{pq} \lambda_{pq}^{\beta/2} \varphi_{pq}. \quad (10)$$

为了求解周期边界条件下的分数阶 CH 方程(9), 基于谱方法的相关理论<sup>[33]</sup>, 我们利用如下的 Fourier 级数来逼近  $\{u_{ij}(t)\}$ , 即

$$F_M^{-1}[\hat{u}(t)](ij) := (P_M u)(x, y, t) = u_{ij}(t) = \sum_{p=-M/2}^{M/2} \sum_{q=-M/2}^{M/2} \hat{u}_{pq} \varphi_{pq}(x_i, y_j). \quad (11)$$

然后, 利用快速 Fourier 变换(FFT)计算离散函数值  $\{u_{ij}(t)\}$  的离散 Fourier 系数  $\{\hat{u}_{pq}(t)\}$ :

$$F_M[u(t)](pq) := \hat{u}_{pq}(t) = \frac{h^2}{C_p^{\text{per}} C_q^{\text{per}} (b-a)^2} \sum_{i=0}^{M-1} \sum_{j=0}^{M-1} u_{ij} \varphi_{pq}(x_i, y_j), \quad (12)$$

其中

$$\begin{cases} \lambda_{pq} = \left(\frac{2p\pi}{b-a}\right)^2 + \left(\frac{2q\pi}{b-a}\right)^2, \\ \varphi_{pq} = \exp\left(\sqrt{-1} \cdot \frac{2p\pi(x-a)}{b-a} + \sqrt{-1} \cdot \frac{2q\pi(y-a)}{b-a}\right), \end{cases} \quad (13)$$

且  $p, q = 0, \pm 1, \pm 2, \dots, \pm M/2$ ,  $\sqrt{-1}$  为虚数单位,  $C_p^{\text{per}}$  和  $C_q^{\text{per}}$  定义为

$$C_r^{\text{per}} = \begin{cases} 2, & |r| = \frac{M}{2}, \\ 1, & |r| < \frac{M}{2}. \end{cases}$$

将式(12)代入式(8)中可得

$$\frac{d\hat{u}_{pq}}{dt} = \frac{\alpha-1}{\alpha}(\hat{u}_{pq} - (\hat{u}_0)_{pq}) + \frac{1}{\alpha}(-\lambda_{pq})(\varepsilon\lambda_{pq}^{\beta/2}\hat{u}_{pq} + f(\hat{u}_{pq})). \quad (14)$$

### 1.3 时间逼近: Crank-Nicolson 格式

取  $N$  个时间节点, 时间步长为  $\tau = T/N$ , 记  $t_n = n\tau$ , 并用  $u_{i,j}^n$  表示  $u(x_i, y_j, t_n)$  的数值近似. 记  $u^{n+1/2} = (u^{n+1} + u^n)/2$ ,  $u_i^n = (u^{n+1} - u^n)/\tau$ , 可得如下的全离散格式:

$$\frac{\hat{u}_{pq}^{n+1} - \hat{u}_{pq}^n}{\tau} = \frac{\alpha - 1}{2\alpha}(\hat{u}_{pq}^{n+1} + \hat{u}_{pq}^n) - \frac{(\alpha - 1)\tau}{\alpha} \hat{u}_0 - \frac{\lambda^{1+\beta/2}}{2\alpha}(\hat{u}_{pq}^{n+1} + \hat{u}_{pq}^n) - \frac{\lambda}{2\alpha\varepsilon}(\hat{f}^{n+1} + \hat{f}^n).$$

由于此数值格式是 Crank-Nicolson 格式, 时间方向的精度为二阶, 此处不再赘述. 将非线性项的具体表达式代入上式, 整理得

$$\left[ 1 - \frac{(\alpha - 1)\tau}{2\alpha} + \frac{\tau\lambda^{1+\beta/2}}{2\alpha} - \frac{\tau\lambda_{pq}}{2\alpha\varepsilon} \right] \hat{u}_{pq}^{n+1} = \left[ 1 + \frac{(\alpha - 1)\tau}{2\alpha} - \frac{\tau\lambda^{1+\beta/2}}{2\alpha} + \frac{\tau\lambda_{pq}}{2\alpha\varepsilon} \right] \hat{u}_{pq}^n - \frac{(\alpha - 1)\tau}{\alpha} \hat{u}_0 - \frac{\tau\lambda_{pq}}{2\alpha\varepsilon}(\hat{u}_{pq}^n)^3 - \frac{\tau\lambda_{pq}}{2\alpha\varepsilon}(\hat{u}_{pq}^{n+1})^3.$$

由于上述格式还存在非线性项, 我们将利用定点迭代来求解, 即对  $k = 1, 2, \dots, K$ , 令  $\hat{u}_{pq}^{n+1,0} = \hat{u}_{pq}^n$ , 得分数阶 CH 方程的数值格式:

$$\hat{u}_{pq}^{n+1,k} = \frac{\left\{ \left[ 1 + \frac{(\alpha - 1)\tau}{2\alpha} - \frac{\tau\lambda^{1+\beta/2}}{2\alpha} + \frac{\tau\lambda_{pq}}{2\alpha\varepsilon} \right] \hat{u}_{pq}^{n,k} - \frac{(\alpha - 1)\tau}{\alpha} \hat{u}_0 - \frac{\tau\lambda_{pq}}{2\alpha\varepsilon}(\hat{u}_{pq}^{n,k})^3 - \frac{\tau\lambda_{pq}}{2\alpha\varepsilon}(\hat{u}_{pq}^{n+1,k-1})^3 \right\}}{1 - \frac{(\alpha - 1)\tau}{2\alpha} + \frac{\tau\lambda^{1+\beta/2}}{2\alpha} - \frac{\tau\lambda_{pq}}{2\alpha\varepsilon}}, \quad (15)$$

此时  $K$  为正整数, 可根据具体情况选取适当的值.

## 2 数值算例

本节中, 我们将利用两个数值算例来验证所得数值格式的有效性. 通过算例 1, 我们给出不同时间、空间分数阶时的误差, 并验证时间方向的收敛阶, 同时呈现不同分数阶、不同时刻的数值解图像; 通过算例 2, 我们验证了本文数值算法满足能量耗散性质和质量守恒律. 为了验证数值解的精度, 现定义  $L^2$  范数意义下的误差  $E_{r_2}^\tau$ , 即

$$E_{r_2}^\tau = \| u^\tau - u^{\tau/2} \|_2;$$

收敛阶

$$R = \log_2(E_{r_2}^\tau/E_{r_2}^{\tau/2}).$$

### 2.1 算例 1

为验证不同分数阶、不同剖分及不同迭代次数下时间方向的误差和收敛阶, 考虑空间区域  $\Omega = [0, 2\pi] \times [0, 2\pi]$  上的二维问题, 初值为

$$u(x, y, 0) = 0.05 \sin x \sin y.$$

边界条件为周期边界条件, 具体参数如下:

$$T = 1, M = 80, \varepsilon = 0.1.$$

表 1 给出了当  $T = 1$  时, 不同分数阶、不同迭代次数及不同剖分下的误差及收敛阶.

表 1 不同分数阶时的  $L^2$  误差及收敛阶

Table 1 The  $L^2$  errors and convergence orders of different fractional orders

$(\alpha, \beta)$	$\tau$	(0.5, 1.4)		(0.9, 1.3)		(0.3, 1.9)		(0.9, 1.9)	
		$E_{r_2}^\tau$	$R$	$E_{r_2}^\tau$	$R$	$E_{r_2}^\tau$	$R$	$E_{r_2}^\tau$	$R$
2	1/200	4.56E-3		8.86E-4		1.82E-3		7.06E-5	
	1/400	1.12E-3	2.029 2	2.21E-4	2.000 4	4.64E-4	1.966 9	1.76E-5	2.000 5
	1/800	2.81E-4	1.992 2	5.53E-5	2.000 2	1.19E-4	1.966 9	4.41E-6	2.000 3
	1/1 600	7.10E-5	1.983 2	1.38E-5	2.000 1	3.03E-5	1.971 3	1.10E-6	2.000 1
	1/3 200	1.79E-5	1.985 3	3.46E-6	2.000 0	7.69E-6	1.980 4	2.76E-7	2.000 1

续表 1

$(\alpha, \beta)$		$(0.5, 1.4)$		$(0.9, 1.3)$		$(0.3, 1.9)$		$(0.9, 1.9)$	
$K$	$\tau$	$E_{r_2}^\tau$	$R$	$E_{r_2}^\tau$	$R$	$E_{r_2}^\tau$	$R$	$E_{r_2}^\tau$	$R$
3	1/200	6.59E-3		9.12E-4		9.64E-5		6.96E-5	
	1/400	1.57E-3	2.067 0	2.28E-4	2.000 6	1.62E-5	2.573 8	1.74E-5	2.000 0
	1/800	3.82E-4	2.041 1	5.70E-5	2.000 2	3.21E-6	2.333 6	4.35E-6	2.000 0
	1/1 600	9.00E-5	2.023 7	1.42E-5	2.000 1	7.84E-7	2.035 6	1.09E-6	2.000 0
	1/3 200	2.33E-5	2.013 0	3.56E-6	2.000 0	2.07E-7	1.921 2	2.72E-7	2.000 0
4	1/200	5.82E-3		9.12E-4		6.81E-5		6.96E-5	
	1/400	1.47E-3	1.986 6	2.28E-4	2.000 4	1.53E-5	2.152 3	1.74E-5	2.000 0
	1/800	3.68E-4	1.995 4	5.70E-5	2.000 1	3.72E-6	2.042 4	4.35E-6	2.000 0
	1/1 600	9.22E-5	1.998 6	1.42E-5	2.000 0	9.21E-7	2.013 0	1.09E-6	2.000 0
	1/3 200	2.31E-5	1.999 6	3.56E-6	2.000 0	2.30E-7	2.004 0	2.72E-7	2.000 0

从表中的数据可以看出,此算法精度较高,时间收敛阶为二阶,也就是说在利用上述数值算法求解分数阶 CH 方程时,Laplace 变换引起的误差较小,还未对数值解造成影响.除此之外,我们还观察到,算法迭代 3 次就可以得到稳态解.下边我们给出不同分数阶、不同时刻的数值解图像(图 1~4),具体参数为

$$M = 100, dt = 1/200, \varepsilon = 0.1, K = 2.$$

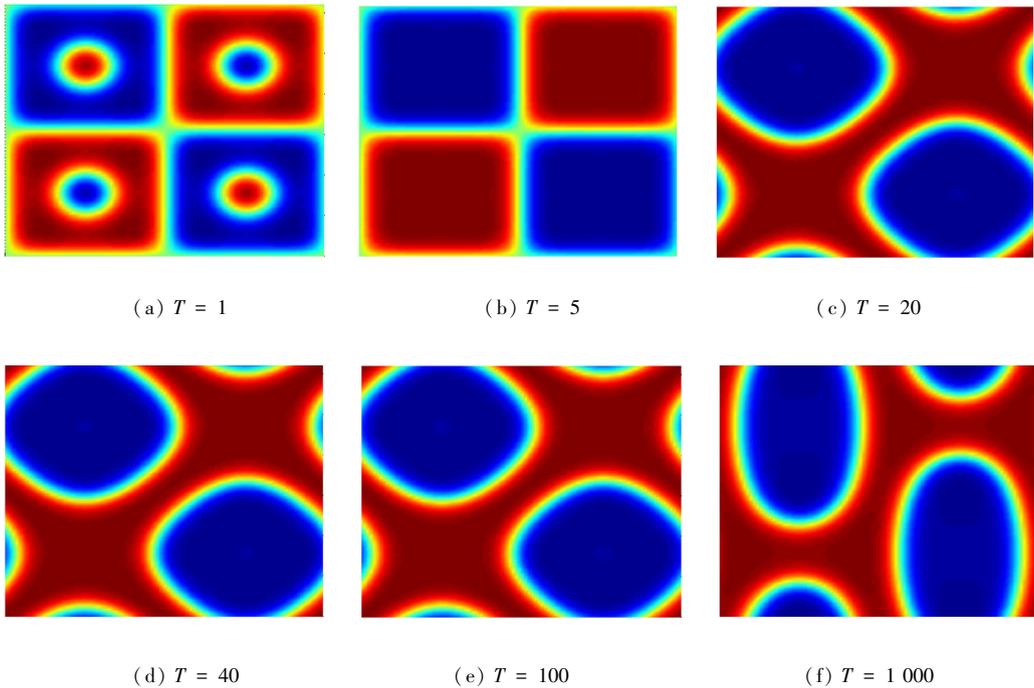


图 1  $\alpha = 0.5, \beta = 1.4$  时,不同时刻的数值解图像

Fig. 1 Numerical solution images for  $\alpha = 0.5, \beta = 1.4$

## 2.2 算例 2

首先,初值仍然选取算例 1 中周期边界条件下的初值,定义如下的能量泛函:

$$E^\beta(\hat{u}^n) = \frac{\varepsilon h^2}{2} \sum_{i=0}^M \sum_{j=0}^M \hat{u}_{ij}^n \lambda_{pq}^{\beta/2} \hat{u}_{ij}^n + \frac{h^2}{4} \sum_{i=0}^M \sum_{j=0}^M ((\hat{u}_{ij}^n)^2 - 1)^2.$$

给出不同时间分数阶与空间分数阶下的能量图像(图 5),具体参数为

$$X = 2\pi, T = 100, M = 80, N = 200, \varepsilon = 0.1, K = 2.$$

现考虑周期边界条件下的非零初值:  $u(x, y) = 0.05 \sin x \sin y + 0.001$ , 其余参数条件同上.定义如下的离散质量:

$$M(\hat{u}_{ij}^n) = h^2 \sum_{i=0}^M \sum_{j=0}^M \hat{u}_{ij}^n.$$

图 6 给出了不同分数阶时的质量与初始质量的误差图.由图易知,能量随着时间的推移呈递减趋势,且时间分数阶和空间分数阶大小会影响能量衰减的速度及达到稳态时的能量值.具体而言,当时间分数阶  $\alpha$  一定时,空间分数阶  $\beta$  越小,能量衰减得越快;当空间分数阶  $\beta$  一定时,时间分数阶  $\alpha$  越大,能量达到稳态的时间越短.除此之外,本文的数值方法满足质量守恒律.

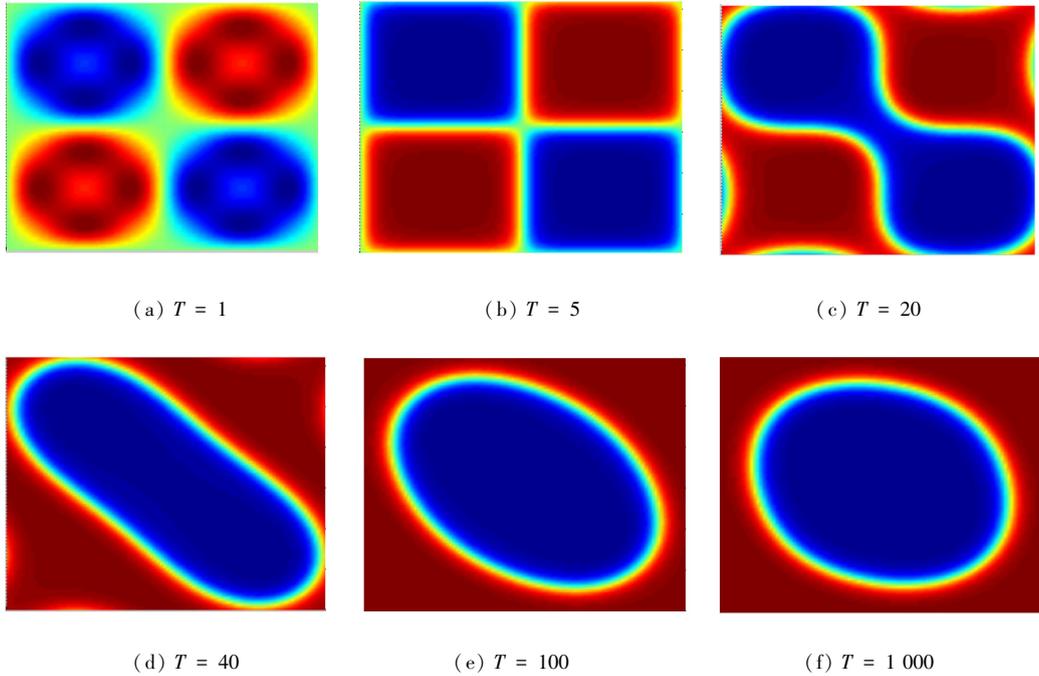


图 2  $\alpha = 0.9, \beta = 1.3$  时,不同时刻的数值解图像

Fig. 2 Numerical solution images for  $\alpha = 0.9, \beta = 1.3$

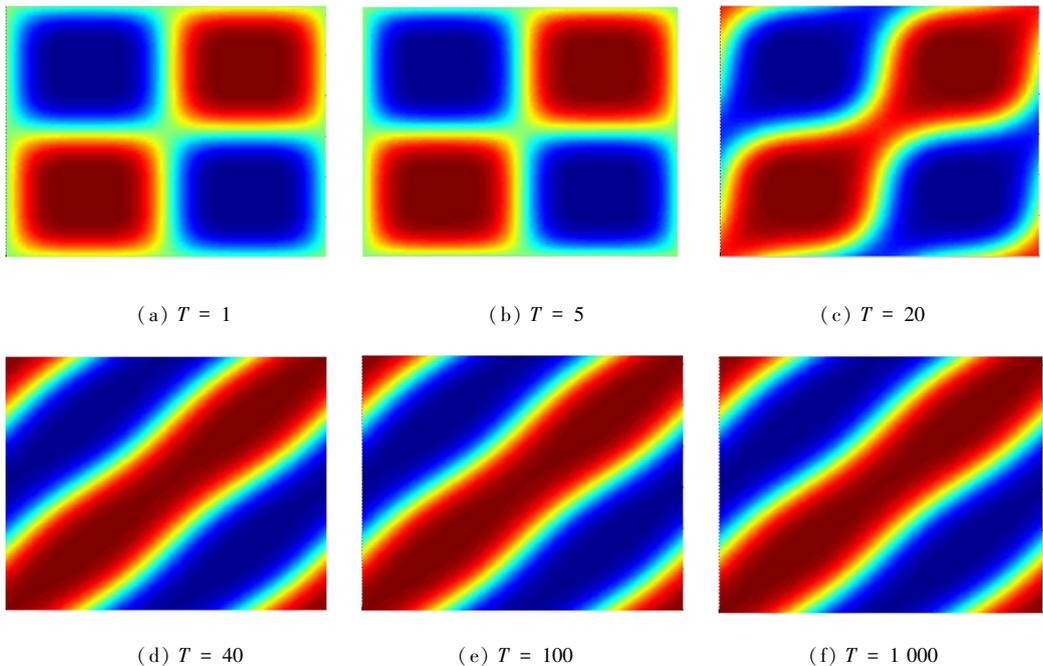


图 3  $\alpha = 0.3, \beta = 1.9$  时,不同时刻的数值解图像

Fig. 3 Numerical solution images for  $\alpha = 0.3, \beta = 1.9$

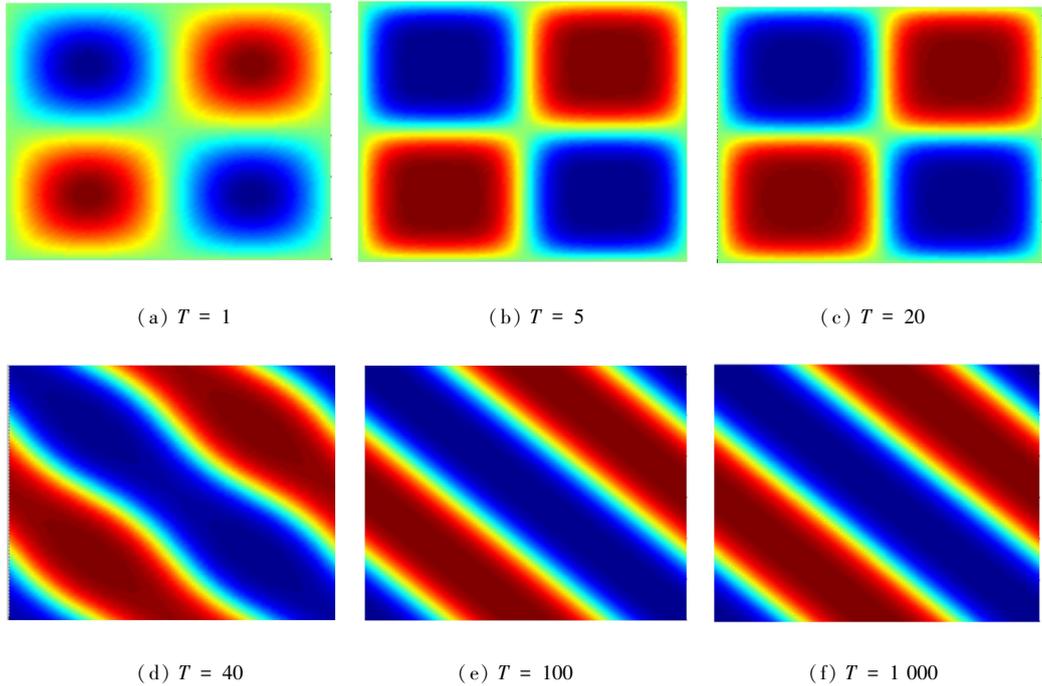


图4  $\alpha = 0.9, \beta = 1.9$  时,不同时刻的数值解图像

Fig. 4 Numerical solution images for  $\alpha = 0.9, \beta = 1.9$

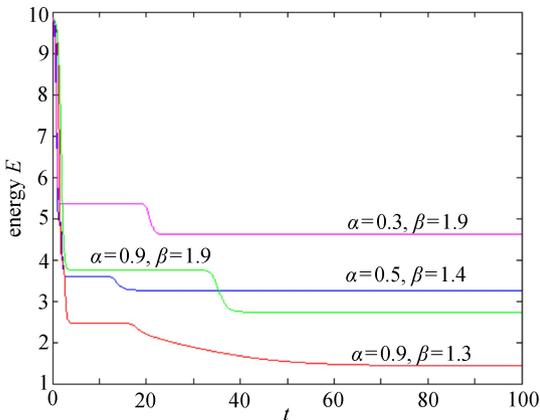


图5 不同分数阶时的能量图像

Fig. 5 Energy change curves of different fractional orders

注 为了解释图中的颜色,读者可以参考本文的电子网页版本。

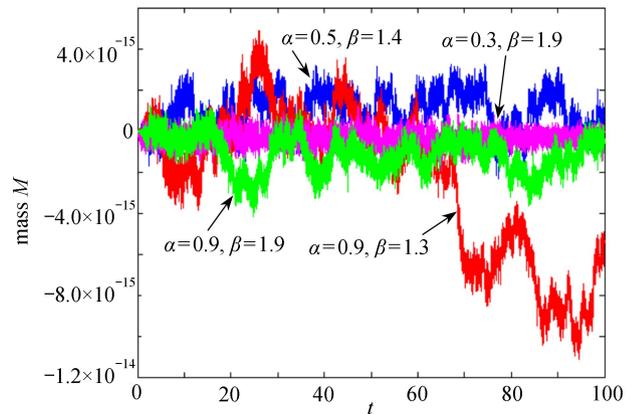


图6 不同分数阶时的质量误差图

Fig. 6 Mass error curves of different fractional orders

### 3 结束语

本文给出了求解分数阶 CH 方程的一个高效数值算法.基于 Laplace 变换,将时空分数阶问题转化为了空间分数阶问题,空间方向利用 Fourier 谱方法,时间方向采用 Crank-Nicolson 格式,得到一个时间二阶的高效数值格式.最后通过数值实验验证了数值格式的有效性,并验证了本文算法满足能量耗散性质和质量守恒.

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