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# Fourier pseudospectral method on generalized sparse grids for the space-fractional Schrödinger equation

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ABSTRACT

In this paper, the time-splitting Fourier pseudospectral method on the generalized sparse grids is applied to solve the space-fractional Schrödinger equation. We give a containment relation between different level-index sets of the generalized sparse grids, and it can be used in designing the reference generalized sparse grids which are finer than other considered grids. Thus the numerical solution on the reference generalized sparse grids can be used as the reference true solution of the equation. Then, the fully discrete algorithm is obtained. In the numerical experiments, we compare the numerical results on the generalized sparse grids with those on the full grids. For the interpolation of the Gaussian multiplied by a factor and for the computation of the Schrödinger equation with two kinds of non-smooth potentials, the advantages of the Fourier pseudospectral method on the generalized sparse grids with the level-index set of parameter $K = 1, 2, 3$ are manifest in the approximation with high resolution. Here the sparsity of the generalized sparse grids will become weak when the parameter $K$ becomes large. Moreover, the advantage of the generalized sparse grids is more pronounced in solving the Schrödinger equation with the higher dimension, the square well potential or the fractional Laplacian.


## 1. Introduction

Consider the $d$-dimensional ($d > 0$) time-dependent space-fractional Schrödinger equation (SFSE) with periodic boundary conditions, i.e.

$$i\frac{\partial}{\partial t}\psi(\mathbf{x},t) = \frac{1}{2}\left(-\Delta\right)^{\alpha/2}\psi + V(\mathbf{x})\psi, \qquad (\mathbf{x},t) \in \mathbb{T}^d \times \mathbb{R}_+, \tag{1.1}$$

where $\psi = \psi(\mathbf{x},t)$ is a complex-valued function and depends on the spatial variable $\mathbf{x} = (x_1, x_2, \ldots, x_d)$ and the time $t$, $i$ is the imaginary unit, $\mathbb{T}^d = \left(\mathbb{R}/2\pi\mathbb{Z}\right)^d$ is a $d$-dimensional torus, and the potential $V(\mathbf{x})$ is a real-valued function defined on $\mathbb{T}^d$. Here, the fractional Laplacian $\left(-\Delta\right)^{\alpha/2}$ is defined as [1]

$$(-\Delta)^{\alpha/2}f(\mathbf{x}) = \sum_{\mathbf{k}\in\mathbb{Z}^d} |\mathbf{k}|_2^{\alpha}\hat{f}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}, \qquad \mathbf{x} \in \mathbb{T}^d, \tag{1.2}$$

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where $\mathbf{k}\cdot\mathbf{x} = k_1x_1 + k_2x_2 + \cdots + k_dx_d$, $|\mathbf{k}|_2^\alpha = \left(k_1^2 + k_2^2 + \cdots + k_d^2\right)^{\frac{\alpha}{2}}$, and

$$\hat{f}(\mathbf{k}) = \frac{1}{(2\pi)^d}\int_{[-\pi,\pi]^d} f(\mathbf{x})e^{-i\mathbf{k}\cdot\mathbf{x}}\mathrm{d}\mathbf{x}, \qquad \mathbf{k}\in\mathbb{Z}^d \tag{1.3}$$

are the Fourier coefficients. In particular, (1.2) is the classical integer Laplacian when $\alpha = 2$.

At present, many numerical results for solving the space-fractional differential equations (SFDEs) are about the finite difference methods [2–7]. The spectral methods with the trigonometric basis [8,9] and the weighted polynomial basis [10,11] have also been used for solving the SFDEs. In fact, the spectral methods have the distinct advantages in computing the SFDEs, since some basis functions of spectral methods are non-local, and this corresponds to the characteristics of the fractional derivatives. Schrödinger equation is the fundamental equation of quantum mechanics. The mathematical theory and the numerical methods about the integer-order Schrödinger equation can be referred to [12–14]. The SFSE was derived by Laskin [15] from the Feynman path integral over Lévy process. Guo, Han and Xin [16] discussed the well-posedness of the SFSE with the period boundary conditions. Moreover, the numerical methods for solving the SFSE are very popular in recent years [3–5,7,9,10].

In this paper, we are interested in the application of the sparse grid methods to the fractional order problems. The sparse grid method was proposed by Smolyak [17] for the numerical integration, and it succeeded in solving the multidimensional problems with bounded mixed derivatives [18]. Yserentant, Griebel and Hamaekers [19,20] researched the finite difference method and the finite element method on the sparse grids for computing the electronic Schrödinger equation. Hallatschek [21] used the hierarchical basis theory to obtain the fast Fourier transform (FFT) on sparse grids. Gradinaru [22] implemented the sparse-grid-FFT by standard template library of C++, and applied the Fourier pseudospectral method on sparse grids to solve the time-dependent Schrödinger equation. He also presented the corresponding error analysis [23]. Meanwhile, Shen and Wang [24] researched the sparse-spectral method with the weighted polynomial basis. Bungartz, Griebel, Hamaekers and Knapek [18,19,25] improved the conventional sparse grids to the generalized sparse grids. Griebel and Hamaekers [26] gave the error estimation of the Fourier interpolation on the generalized sparse grids. However, as far as we know, there was no relevant literature about the numerical methods on the sparse grids for computing the SFDEs. It is worth noting that, the mathematical properties of the SFDEs are quite different from those of the integer-order differential equations, especially for multidimensional problems. The properties of the high frequency components in the solutions of the SFDEs may not be the same as those of the integer-order differential equations. Therefore, until the effective numerical experiments are given, we are not sure whether the numerical methods on the sparse grids are suitable for computing the fractional-order problems, although these methods have achieved the great advantages in the corresponding integer-order problems.

The rest of paper is organized as follows.

In Section 2, we briefly introduce the generalized sparse grids and the fast Fourier transformation on the hierarchical basis. Moreover, we give some estimation for the containing relation between different level-index sets.

In Section 3, we obtain the fully discrete algorithm of the Fourier pseudospectral method on the generalized sparse grids for solving the SFSE.

In Section 4, we apply this algorithm to two SFSE problems with the harmonic potential and the square well potential. For different dimensions and different space-derivative orders, the computational errors are presented in the form of figures. Meanwhile, we discuss the computational results obtained by this algorithm with different level-index sets.

In the final section, we give the conclusion.

## 2. Fourier interpolation on the generalized sparse grids

Let

$$G_0 = \{-\pi\}, \quad G_1 = \{0\},$$
$$G_l = \left\{(2k+1)\frac{2\pi}{2^l} - \pi \ : \ k = 0, 1, \ldots, 2^{l-1}-1\right\}, \quad l = 2, 3, \ldots,$$

and

$$S_0 = \{0\}, \quad S_1 = \{1\},$$
$$S_l = \left\{\sigma(k) \ : \ k = 2^{l-1}, 2^{l-1}+1, \ldots, 2^l - 1\right\}, \quad l = 2, 3, \ldots,$$

where

$$\sigma(k) = \begin{cases} -k/2, & \text{if } k \text{ is even}, \\ (k+1)/2, & \text{if } k \text{ is odd}, \end{cases} \qquad k\in\mathbb{N}_0,$$

and $\mathbb{N}_0$ denotes the natural number set including "0". The generalized sparse grid is defined as

$$\mathcal{G}_\mathcal{A} = \left\{\mathbf{x}\in\mathbb{R}^d \ : \ x_j \in G_{l_j}, \mathbf{l}\in\mathcal{A}, j = 0, 1, \ldots, d-1\right\}, \tag{2.1}$$

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