Advances in Applied Mathematics and Mechanics
Adv. Appl. Math. Mech., Vol. **17**, No. 6, pp. 1789-1812

DOI: 10.4208/aamm.OA-2023-0217
December 2025

Two Novel Space-Time Polynomial Particular Solutions Methods for the Time-Dependent Schrödinger Equation

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Received 16 August 2023; Accepted (in revised version) 3 November 2023

Abstract. The conventional method of polynomial particular solutions is only applicable to partial differential equations on the real number field. Building on this method, this paper proposes two novel approaches for numerical simulation of the time-dependent Schrödinger equation. Under the assumption of treating the time variable as an ordinary spatial variable, the first approach approximates the real and imaginary parts of the equation using two different sets of linear combinations, which are then substituted into the corresponding original governing equations to form a coupled differential equation. The second approach is derived based on the basic form of complex coefficient partial differential equations and involves polynomial particular solutions with imaginary terms. Using the same numerical examples, compared to conventional finite difference method, Fourier spectral method and radial basis function collocation method, this algorithm's stability is not limited by the grid ratio of the time step and spatial step. It is not only simple and feasible but also suitable for solving high-dimensional problems.

AMS subject classifications: 65M06, 65M70

Key words: Schrödinger equation, space-time methods, meshless methods, method of polynomial particular solutions.

1 Introduction

The Schrödinger equation is a mathematical equation in quantum mechanics that describes the evolution of the wave function over time [1], incorporating information about the position, momentum, and energy of a particle. Its solutions are important in many fields such as the development of new quantum technologies, the design and optimization of materials, and the understanding of the properties and behavior of the microcosmic world [2]. The solutions to the Schrödinger equation can be obtained through either

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analytical or numerical methods [3]. However, obtaining accurate solutions for complex systems can be challenging, making numerical methods more practical. With the development of numerical methods and advances in computer performance, existing numerical methods are becoming increasingly effective in dealing with the time-dependent Schrödinger equation [4].

As is known, the conventional approach to solving the time-dependent Schrödinger equation is to discretize the problem into a finite number of points or regions and then solve algebraic equations iteratively. From the early days of using finite difference method [5] to solve one-dimensional nonlocal potentials, which are simple and intuitive, there have been both extensions and limitations when nonlocal potentials act on a system. Firstly, nonlocal potentials require more memory to store potential energy values, and as a result, the calculated eigenvalues of energy will be changed accordingly. To solve this problem, the potential must be designed as a function with specific periodicity or smoothness. Secondly, it is crucial to note that finite difference methods may suffer from numerical instability due to rounding errors and large time steps, and they are constrained by the real-space potential defined at grid points. Overall, finite difference methods are a straightforward and easy-to-implement method for solving the time-dependent Schrödinger equation, but when dealing with nonlocal potentials, one needs to balance computational efficiency and numerical stability and use other methods to better handle boundary problems [6–8]. Subsequently, there emerged the pseudospectral method based on Chebyshev polynomials, which represented the time evolution operator as an exponential function and used fast Fourier transforms for computation [9–12]. This method has excellent stability and is more capable of handling nonlocal potentials, not only shortening computation time but also providing high accuracy and scalability. However, this method is not suitable for high-dimensional problems and is prone to numerical oscillations. Since it requires Fourier transformations and inverse transformations, it consumes more computational resources. Additionally, the finite element method discretizes the wave function into small triangular or quadrilateral elements, which are accurate and convenient for handling complex-shaped calculation domains [13–16]. However, it requires a large amount of operational calculations and is difficult to divide meshes for irregular shapes and complex domains. As for the recently emerging meshless methods, which use point cloud data structure to represent the solution domain and approximate the wave function with moving least squares interpolation, its biggest advantage is that it completely eliminates the need for mesh generation, solves the problem of mesh deformation and movement, and is conducive to optimization and control and is applicable to high-dimensional problems. However, its shortcomings are also obvious. First, we must choose appropriate kernel and interpolation functions [17–20], and the stability, computational resources, and computational time of the algorithm are also worth exploring. These methods have their advantages and limitations, so it is necessary to analyze and optimize them according to specific problems in order to obtain the best numerical solution.

The main work of this paper is to cleverly use the method of polynomial particu-