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On the rational second kind Chebyshev pseudospectral method for the solution of the Thomas–Fermi equation over an infinite interval

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ABSTRACT

In this paper, we propose a pseudospectral method for solving the Thomas–Fermi equation which is a nonlinear singular ordinary differential equation on a semi-infinite interval. This approach is based on the rational second kind Chebyshev pseudospectral method that is indeed a combination of tau and collocation methods. This method reduces the solution of this problem to the solution of a system of algebraic equations. The slope at origin is provided with high accuracy. Comparison with some numerical solutions shows that the present solution is effective and highly accurate.

1. Introduction

A number of problems arising in science and engineering are set in semi-infinite domains. We can apply different spectral methods that are used to solve problems in semi-infinite domains. The first approach is using Laguerre or Hermite polynomials [1–5]. The second approach is replacing the semi-infinite domain with $[0, L]$ interval by choosing L, sufficiently large. This method is named domain truncation [6,7]. The third approach is reformulating original problem in the semi-infinite domain to singular problem in the bounded domain by variable transformation and then using the Jacobi polynomials to approximate the resulting singular problem [8–12]. The fourth approach of the spectral method is based on rational orthogonal functions. Boyd [13,14] defined a new spectral basis, named rational Chebyshev functions on the semi-infinite interval, by mapping to the Chebyshev polynomials. Guo et al. [15] introduced a new set of rational Legendre functions which are mutually orthogonal in $L^2(0, +\infty)$. They applied a spectral scheme using the rational Legendre functions for solving the Korteweg–de Vries equation on the half line. Boyd et al. [16] applied pseudospectral methods on a semi-infinite interval and compared rational Chebyshev, Laguerre and mapped Fourier sine.

The authors of [17–19] applied the spectral method to solve nonlinear ordinary differential equations on semi-infinite intervals. Their approach was based on a rational Tau method. They obtained the operational matrices of derivative and product of rational Chebyshev and Legendre functions and then they applied these matrices together with the Tau method to reduce the solution of these problems to the solution of the system of algebraic equations. Furthermore, the authors of [20,21] introduced the rational second and third kind Chebyshev tau method for solving the Lane–Emden equation and Volterra's population model as nonlinear differential equations over the infinite interval. In [22], rational second kind Chebyshev bases

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and Galerkin method are used to obtain the approximate solution of a system of high-order integro-differential equations on the semi-infinite interval.

One of the most important nonlinear singular ordinary differential equations that occurs in a semi-infinite interval is the Thomas–Fermi equation, as follows [23,24]:

$$\frac{d^2y}{dx^2} = \frac{1}{\sqrt{x}} y^{\frac{3}{2}}(x), \quad x \geqslant 0, \tag{1}$$

which appears in the problem of determining the effective nuclear charge in heavy atoms. Boundary conditions for this equation are as follows:

$$y(0) = 1, \qquad \lim_{x\to\infty} y(x) = 0. \tag{2}$$

The Thomas–Fermi equation is useful for calculating form factors and for obtaining effective potentials which can be used as initial trial potentials in self-consistent field calculations. For an understanding of the early developments of the Thomas–Fermi equation, we refer the reader to see the review [25], which especially pointed out the considerable contributions to this field made by Fermi and Majorana.

The Thomas–Fermi problem has been solved by different techniques. The authors of [26–28] used a perturbative approach to determine analytic solutions for the Thomas–Fermi equation. Bender et al. [26] replaced the right-hand side of this equation by one which contains the parameter δ, i.e., $y''(x) = y(x)\left(\frac{y(x)}{x}\right)^{\delta}$; the potential is then expanded in a power series in δ

$$y = y_0 + \delta y_1 + \delta^2 y_2 + \delta^3 y_3 + \cdots. \tag{3}$$

This procedure reduced Eq. (1) into a set of linear equations with associated boundary conditions. Laurenzi [27] applied a perturbative method by combining it with an alternate choice of the nonlinear term of Eq. (1) to produce a rapidly converging analytic solution. Cedillo [28] wrote Eq. (1) in terms of density and then the δ-expansion was employed to obtain an absolute converging series of equations. Adomian [29] applied the decomposition method for solving the Thomas–Fermi equation and then Wazwaz [30] proposed a non-perturbative approximate solution to this equation by using the modified decomposition method in a direct manner without any need to a perturbative expansion or restrictive assumptions. He combined the series obtained with the Padé approximation which provided a promising tool to handle problems on an unbounded domain. Liao [31] solved the Thomas–Fermi equation by the homotopy analysis method. This method provided a convenient way to control the convergence of approximation series and adjusted convergence regions when necessary, which was a fundamental qualitative difference in analysis between the homotopy analysis method and all other reported analytic techniques. Khan [32] used the homotopy analysis method with a new and better transformation which improved the results in comparison with Liao's work. In [33], the quasilinearization approach was applied for solving Eq. (1). This method approximated the solution of a nonlinear differential equation by treating the nonlinear terms as a perturbation about the linear ones, and unlike perturbation theories it is not based on the existence of some kind of a small parameter. Ramos [34] presented two piecewise quasilinearization methods for the numerical solution of Eq. (1). Both methods were based on the piecewise linearization of ordinary differential equations. The first method (C1-linearization) provided global smooth solutions, whereas the second one (C0-linearization) provided continuous solutions. Yao [34] solved the Thomas–Fermi equation by an analytic technique named the homotopy analysis method with a more generalized set of basis function, and consequential auxiliary linear operator was introduced to provide a series solution. Zhu et al. [35] approximated the original Thomas–Fermi equation by a nonlinear free boundary value problem. They then used an iterative method to solve the free boundary value problem. Parand et al. [36] investigated the Sinc-collocation method on the half-line for solving Eq. (1) by using Sinc functions. Similar, for a singular boundary-value problem we refer to.

In this paper, we introduce a combination of tau and pseudospectral methods based on rational second kind Chebyshev (RSC) functions. The proposed method requires the definition of RSC functions, operational matrix of derivative and rational second kind Chebyshev–Gauss collocation points and weights. The application of the method to the Thomas–Fermi equation leads to a nonlinear algebraic system. We employed this method to the Thomas–Fermi equation because first, it is easy to apply and numerically achieve spectral convergence; second, because of singularity in this equation this method can handle this problem; and third, the limit of the RSC functions at infinity is computable and thus the boundary conditions at infinity can easily be handled.

This paper is arranged as follows: in Section 2, we describe the formulation and some properties of rational second kind Chebyshev functions required for our subsequent development. Section 3 summarizes the application of this method for solving the Thomas–Fermi equation and a comparison is made with existing methods in the literature. The conclusions are described in the final section.

2. Properties of RSC functions

In this section, we present some properties of rational second kind Chebyshev functions and introduce the rational second kind Chebyshev pseudospectral approach.