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The Sinc-collocation method for solving the Thomas–Fermi equation

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ABSTRACT

A numerical technique for solving nonlinear ordinary differential equations on a semi-infinite interval is presented. We solve the Thomas–Fermi equation by the Sinc-Collocation method that converges to the solution at an exponential rate. This method is utilized to reduce the nonlinear ordinary differential equation to some algebraic equations. This method is easy to implement and yields very accurate results.

1. Introduction

Recently, spectral methods [1,2] have been successfully applied in the approximation of boundary value problems defined in the semi-infinite domains. We can apply different approaches using spectral methods to solve problems in semi-infinite domains. Various spectral methods for treating semi-infinite domains have been proposed. One approach is using Laguerre polynomials [3–6]. A second approach is reformulating the original problem in the semi-infinite domain to a singular problem in a bounded domain by variable transformation and then using the Jacobi polynomials to approximate the resulting singular problem [7–9]. A third approach of the spectral method is based on rational orthogonal functions, for example, Christov [10] and Boyd [11,12] developed some spectral methods on unbounded intervals by using mutually orthogonal systems of rational functions. Boyd [12] defined a new spectral basis, named rational Chebyshev functions on the semi-infinite interval, by mapping it to the Chebyshev polynomials [13]. Guo et al. [14] proposed and analyzed a set of Legendre rational functions which are mutually orthogonal in ${L_\chi}^2(0,\infty)$ with a non-uniform weight function $\chi(x) = (x+1)^{-2}$. Parand et al. [15–19] applied the rational Chebyshev, rational Legendre and rational scaled generalized Laguerre functions with tau [20,21] and collocation methods to solve nonlinear ordinary differential equations on semi-infinite intervals. A fourth approach is replacing the semi-infinite domain with $[0, L]$ interval by choosing L, sufficiently large, this method is named as the domain truncation [22].

The Sinc-collocation and Sinc–Galerkin methods for solving differential equations are based on Sinc approximation [23]. In this paper, we investigate the Sinc-collocation [24,25] method on the half line by using Sinc functions. The Sinc-collocation

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method for the numerical solution of the initial value problems is developed in [26] and it is approved that it converges to the solution at an exponential rate. In [27,28] the Sinc-collocation method is discussed for solving the Blasius and Planar Coulomb Schrödinger equations on the half line. The Sinc–Galerkin method was applied widely by [29–31]. The author of [29] applied this method to solve certain class of singular two-point boundary value problems and expressed the exact solution of the differential equations via the use of Green's functions as an integral type. Saadatmandi et al. [30] applied the Sinc–Galerkin method for solving nonlinear two-point boundary value problems [32] for the second order differential equations.

2. The Thomas–Fermi equation

The Thomas–Fermi theory establishes a functional relation between the energy of an electronic system, E, and the electronic density, ρ, namely,

$$E[\rho] = \frac{9}{10B}\int \rho(r)d\tau + \frac{1}{2}\int \frac{\rho(r)\rho(r')}{|r-r'|}d\tau' d\tau + \int \rho(r)\nu(r)d\tau, \tag{2.1}$$

where $\nu(r)$ is the external potential and $B = 3(3\pi^2)^{-\frac{2}{3}}$. The density can be obtained by minimizing the energy functional with respect to ρ, subject to the normalization restriction $\int \rho(r)d\tau = N$ where N is a number of electrons [33]. Then the density must satisfy the following integral equation:

$$\frac{3}{2B}\rho(r)^{\frac{2}{3}} + \int \frac{\rho(r')}{|r-r'|}d\tau' + \nu(r) = \mu, \tag{2.2}$$

where μ is the Lagrange multiplier related to the normalization restriction. Poisson's equation can be used to remove the density, and a change of variables leads to the Thomas–Fermi equation

$$\frac{d^2y}{dx^2} = \frac{1}{\sqrt{x}}y^{\frac{3}{2}}(x), \tag{2.3}$$

with boundary conditions as follows:

$$y(0) = 1, \qquad \lim_{x\to\infty} y(x) = 0. \tag{2.4}$$

This equation describes the charge density in atoms of high atomic number and appears in the problem of determining the effective of nuclear charge in heavy atoms [34,35]. It is useful for calculating form-factors and for obtaining effective potentials which can be used as initial trial potentials in self-consistent field calculations. It is also applicable to the study of nucleons in the atom and electrons in the metal. If we use the Runge–Kutta method [36] to solve Eq. (2.3) it can be found numerically with great difficulty, in that, to integrate from $x = 0$ we must assume a value for $y'(0)$, if $y'(0)$ is chosen too small, the solution will cross below the x axis at some finite values of x and becomes complex and if $y'(0)$ is chosen too large the solution will eventually become singular at some finite values of x [37]. It is long known that the solution of this equation is very sensitive to a value of the first derivative at zero which ensures smooth and monotonic decay from $y(0) = 1$ to $y(\infty) = 0$ as demanded by boundary conditions [38]. Cedillo [33] wrote the Thomas–Fermi equation in terms of density and then the δ-expansion was employed to obtain an absolutely convergent series of equations. Mandelzweig and Tabakin [39] employed a quasilinearization method to solve the Thomas–Fermi equation written as $y'' = x^{-1/2}y^{3/2}$ for $0 \le x \le 40$ by means of a quasilinearization method starting with the initial guess $y_0(x) = 1$, and showed that the convergence starts at the boundaries and expands with each iteration to a wider range of values of x.

In this paper we approximate $y(x)$ by the Sinc-collocation method because first, it is easy to apply and numerically achieve exponential convergence, second, because of singularity in this equation Sinc functions can handle this problem, third, the limit of the Sinc function at infinity is zero and thus one of the boundary conditions in Thomas–Fermi equation implicitly becomes true.

The organization of this paper is as follows: in Section 3, we explain the formulation of Sinc functions required for our subsequent development. In Section 4, we summarize the application of the method of Sinc functions for solving the Thomas–Fermi equation and comparing it with the existing methods in the literature. Section 5 is devoted to summary and conclusions.

3. Sinc function properties

The Sinc function is defined for all $x \in R$ by

$$\mathrm{sinc(x)} = \begin{cases} \dfrac{\sin(\pi \mathrm{x})}{\pi \mathrm{x}}, & \mathrm{x} \neq 0, \\ 1, & \mathrm{x} = 0. \end{cases} \tag{3.1}$$